

Figure 1

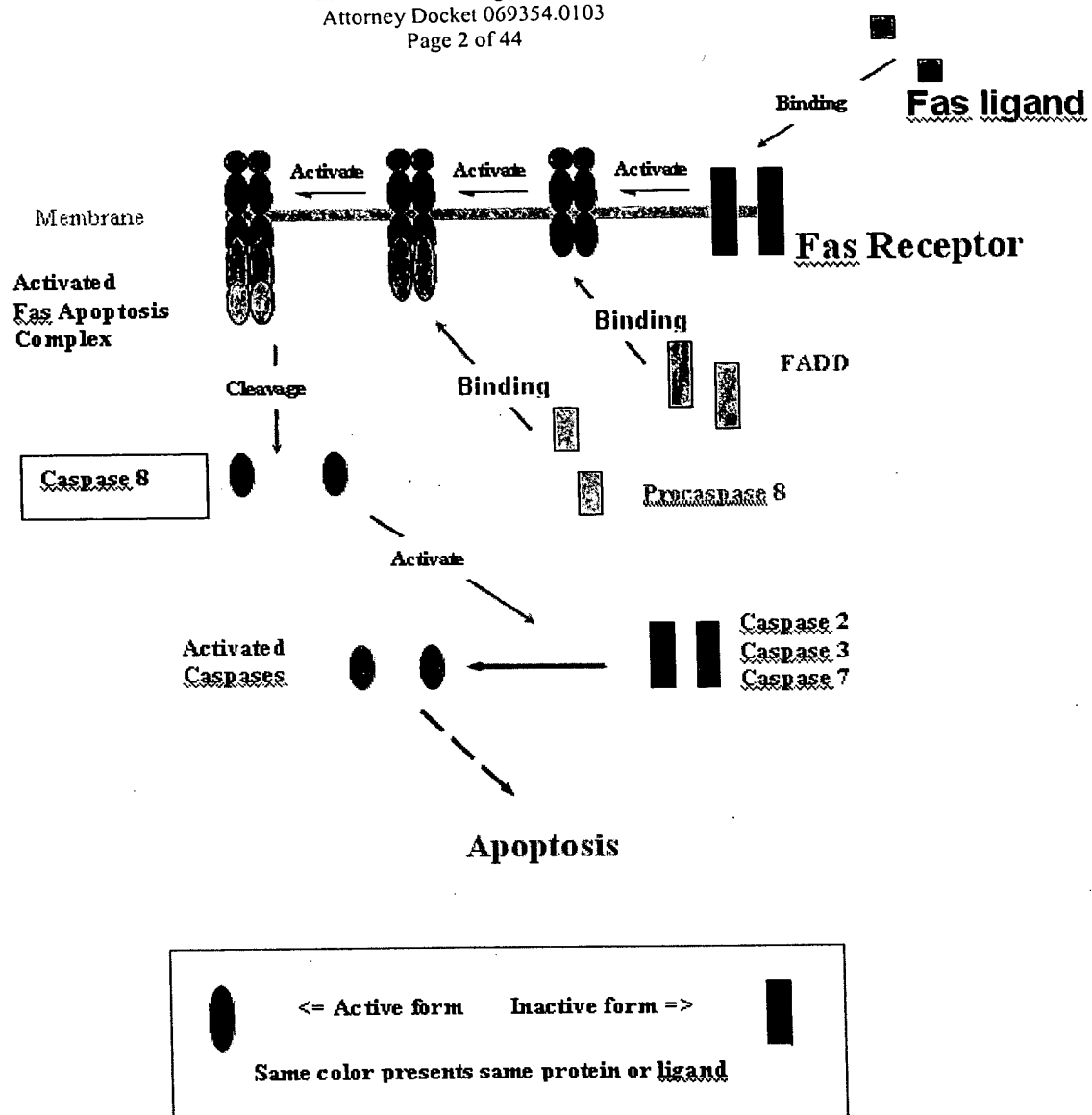


Figure 2

**Methods for Simulation of Biological and/or
Chemical Reaction Pathway, Biomolecules and
Nano-Molecular Systems**

Inventors: Yu Zong Chen et al.

Attorney Docket 069354.0103

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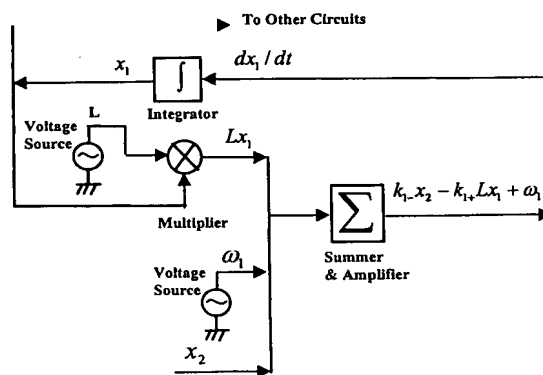


Figure 3A

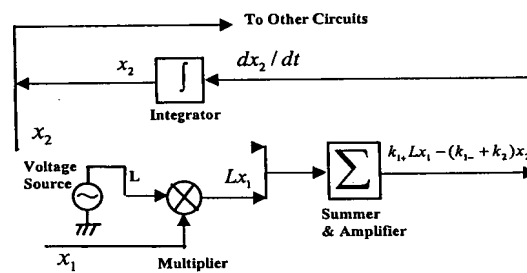


Figure 3B

***Methods for Simulation of Biological and/or
Chemical Reaction Pathway, Biomolecules and
Nano-Molecular Systems***

Inventors: Yu Zong Chen et al.

Attorney Docket 069354.0103

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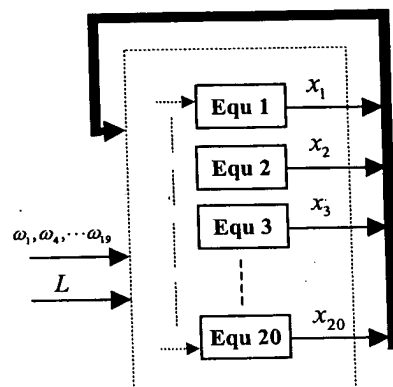


Figure 4

*Methods for Simulation of Biological and/or
Chemical Reaction Pathway, Biomolecules and
Nano-Molecular Systems*
Inventors: Yu Zong Chen et al.
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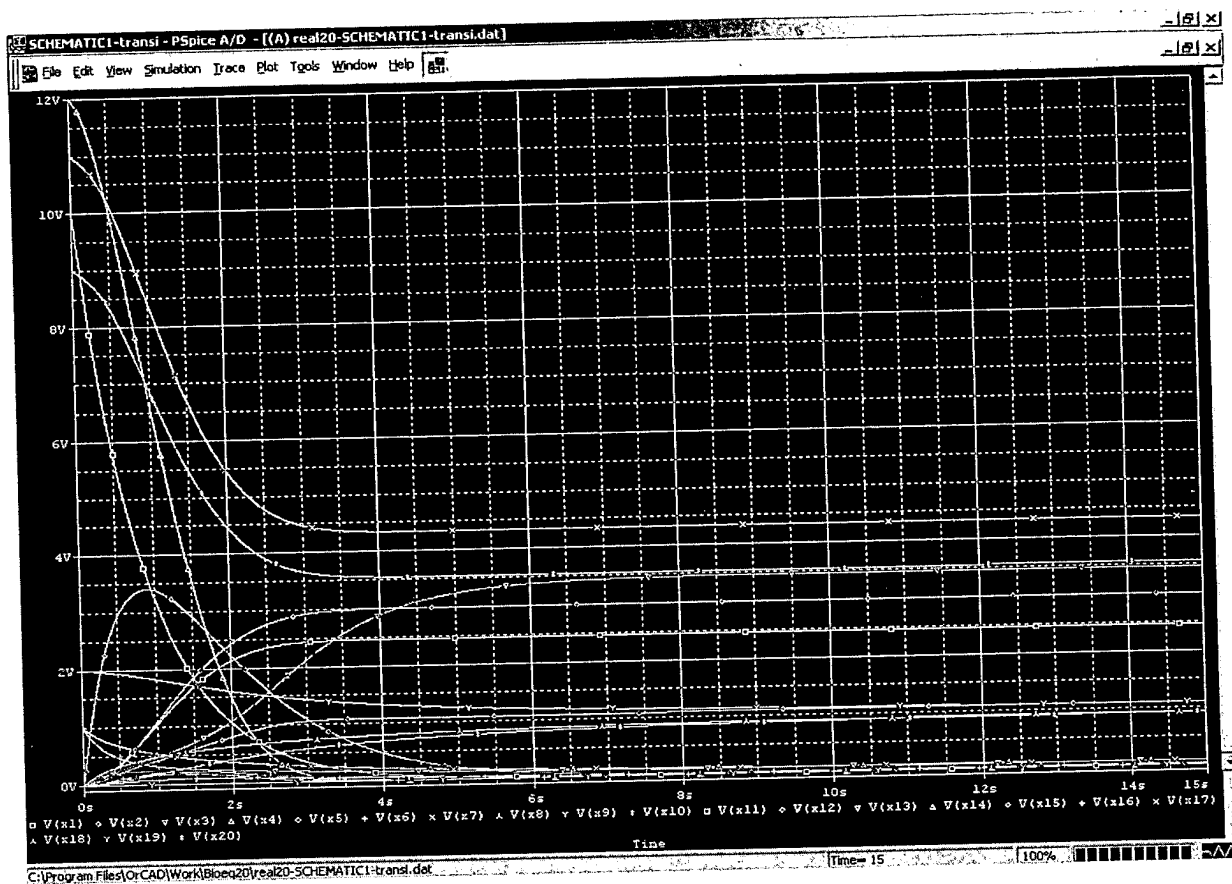


Figure 5

*Methods for Simulation of Biological and/or
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Nano-Molecular Systems*

Inventors: Yu Zong Chen et al.

Attorney Docket 069354.0103

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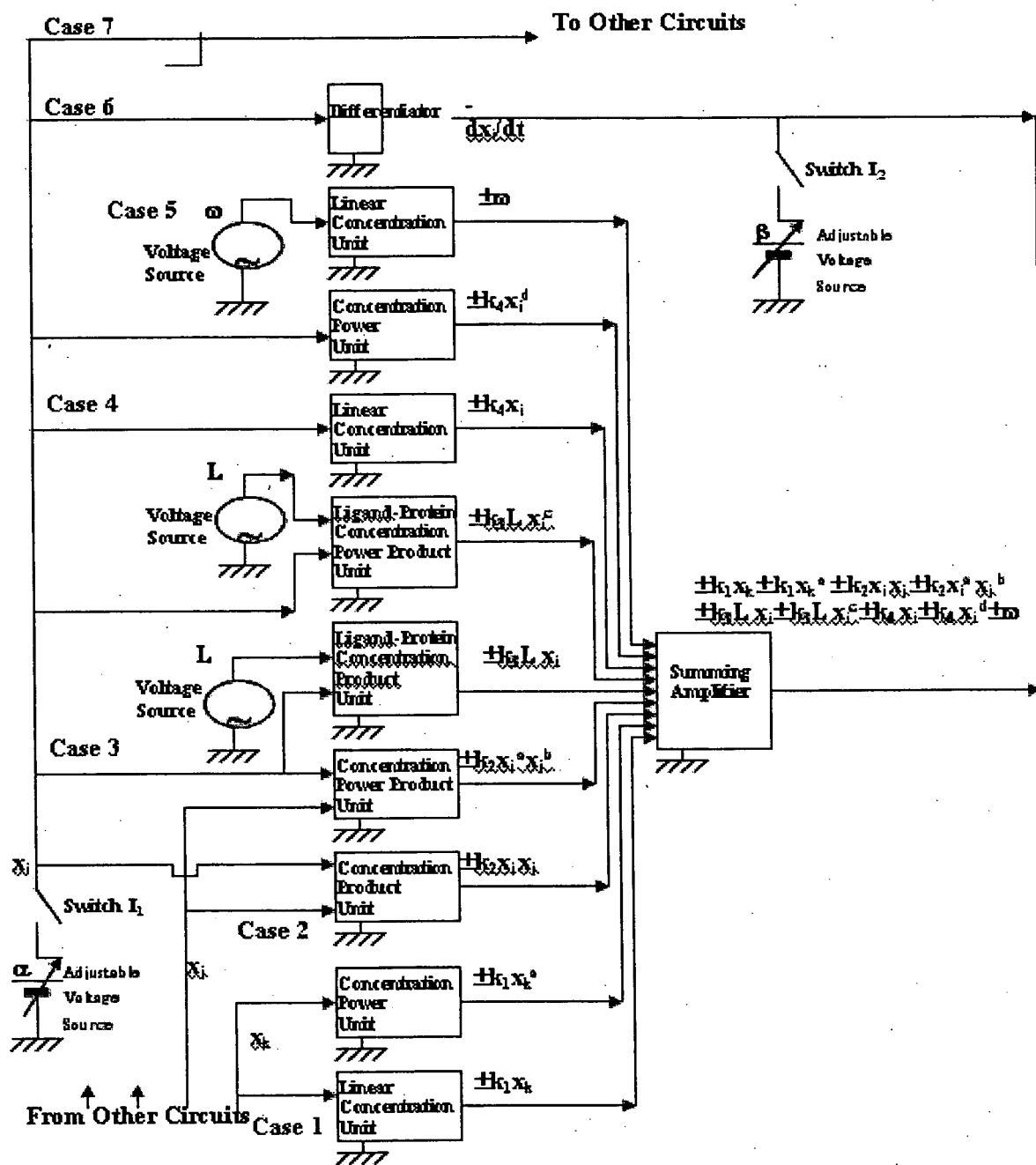


Figure 6

*Methods for Simulation of Biological and/or
Chemical Reaction Pathway, Biomolecules and
Nano-Molecular Systems*

Inventors: Yu Zong Chen et al.

Attorney Docket 069354.0103

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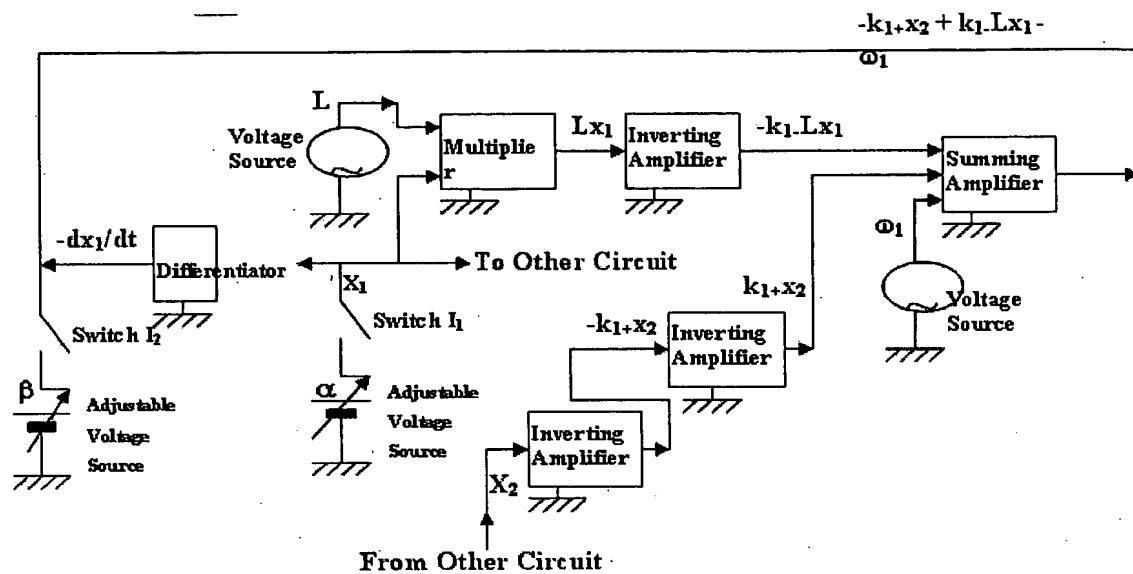


Figure 7

*Methods for Simulation of Biological and/or
Chemical Reaction Pathway, Biomolecules and
Nano-Molecular Systems*

Inventors: Yu Zong Chen et al.

Attorney Docket 069354.0103

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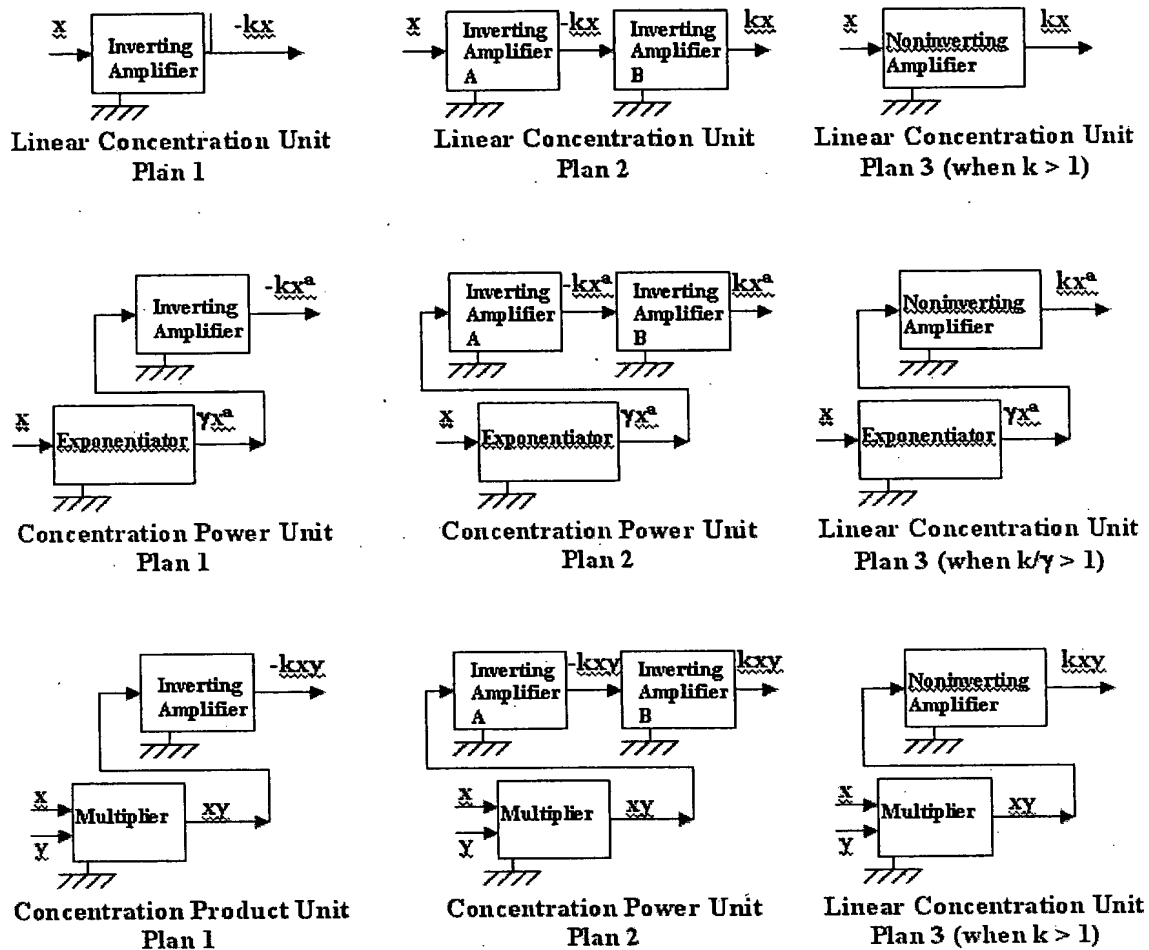
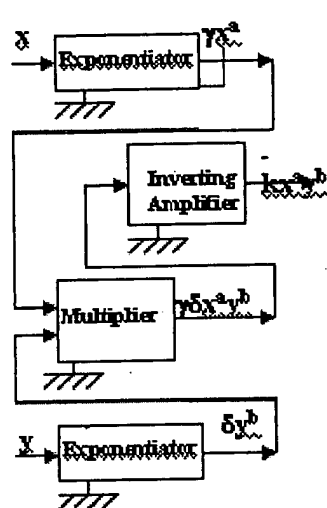
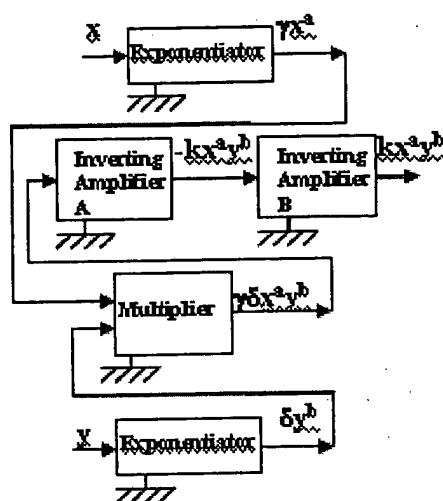


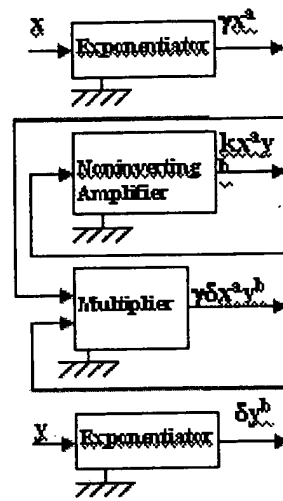
Figure 8



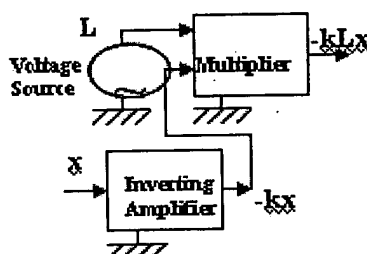
Concentration Power
Product Unit
Plan 1



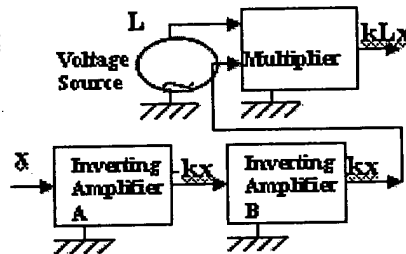
Concentration Power
Product Unit
Plan 2



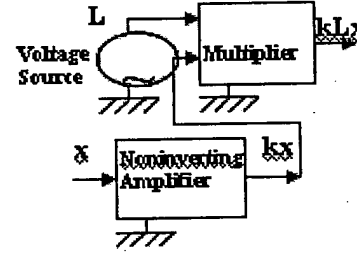
Concentration Power
Product Unit
Plan 3 (when $k/\gamma\delta > 1$)



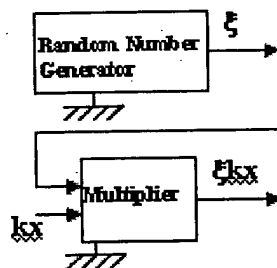
Ligand-Protein
Concentration Product Unit
Plan 1



Ligand-Protein
Concentration Product Unit
Plan 2

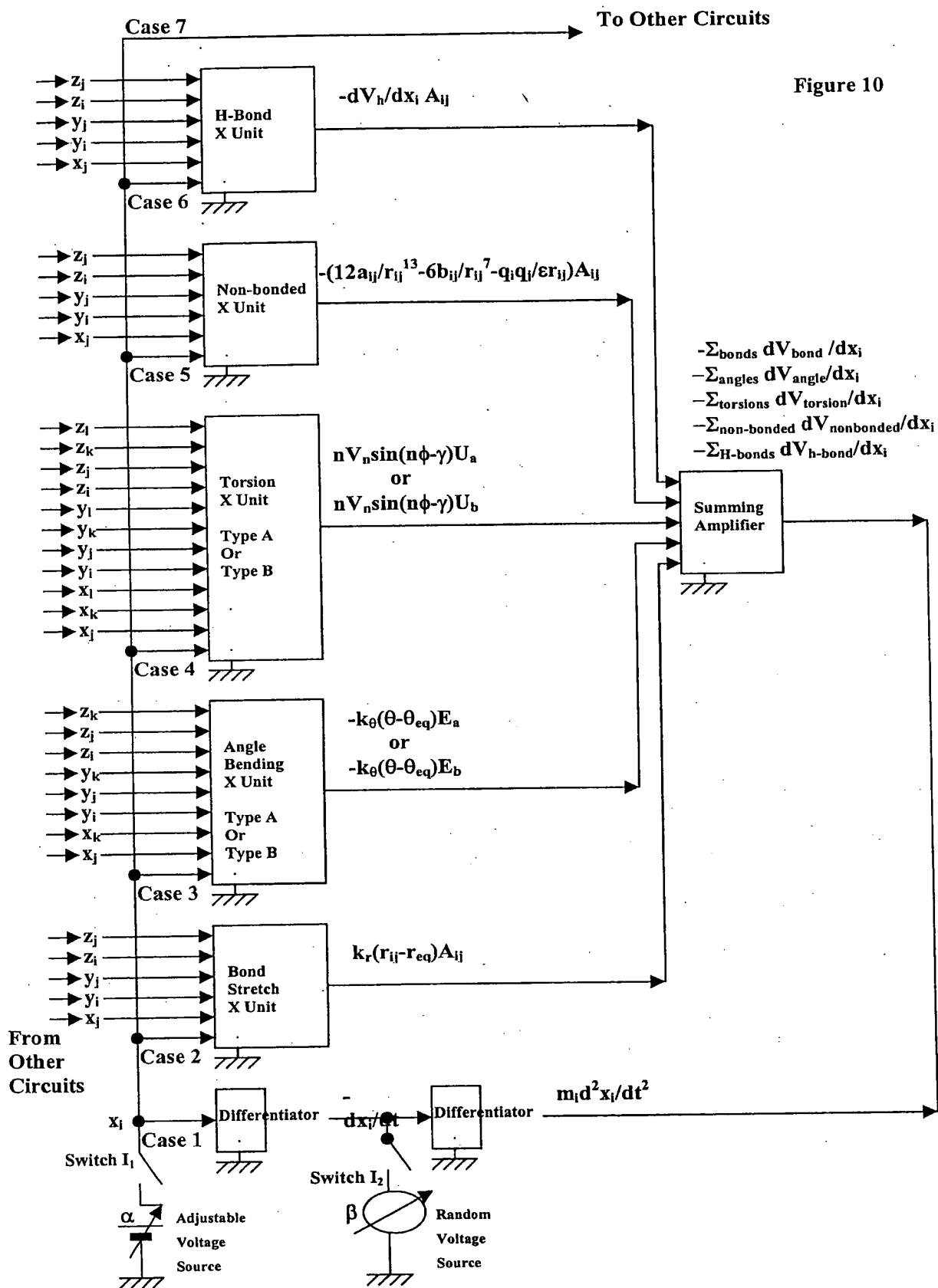


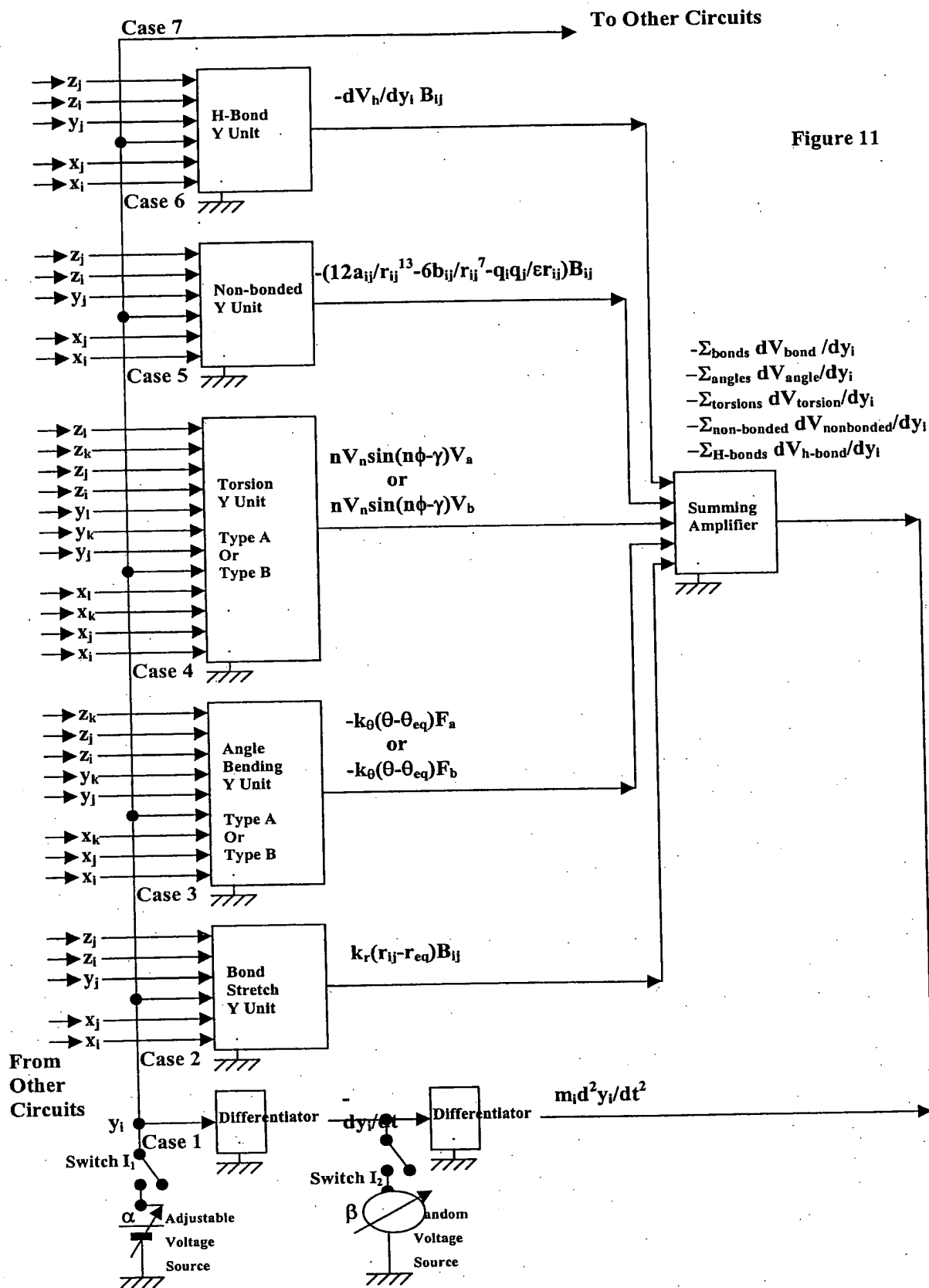
Ligand-Protein
Concentration Product Unit
Plan 3 (when $k > 1$)



Stochastic Rate Constant
Generator unit

Figure 9



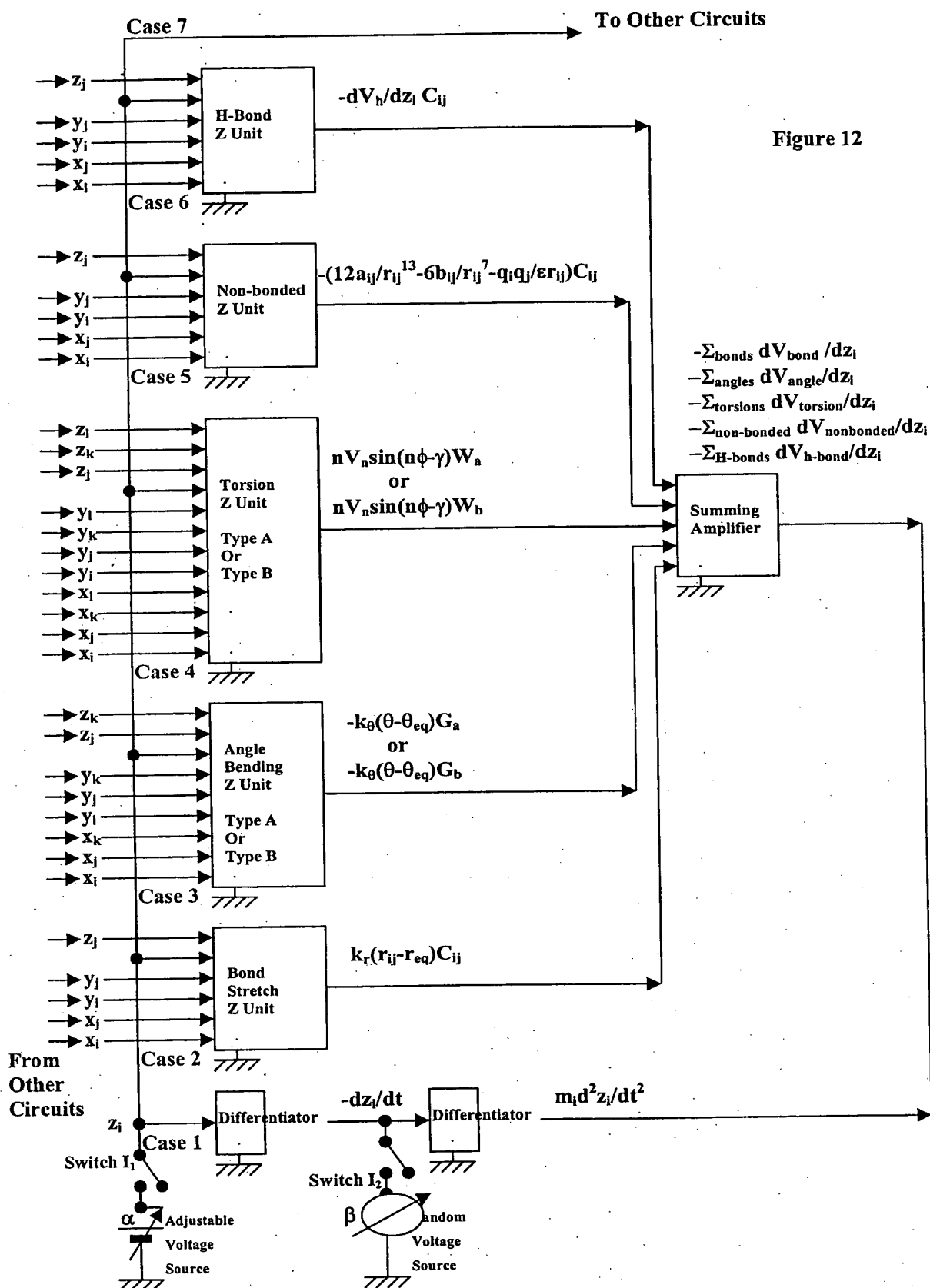


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**Illustration of the Circuit Group
For an Amino Acid
(Bond Stretch Connections)**

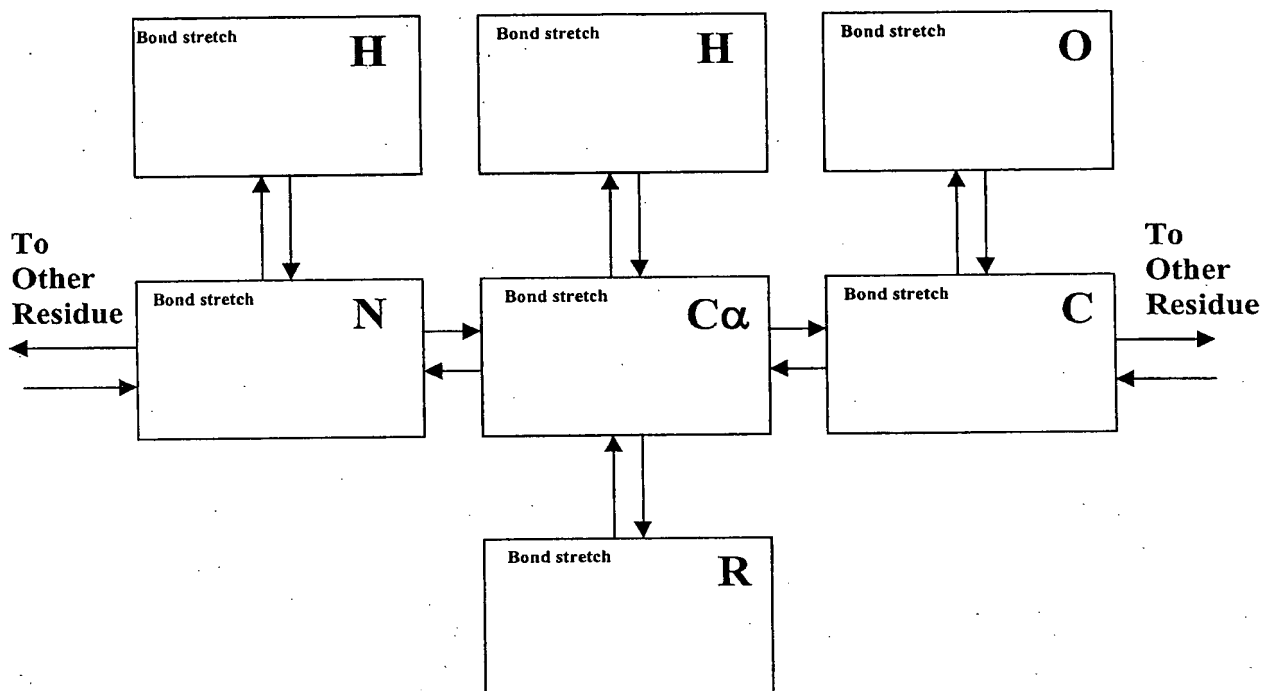


Figure 13

**Illustration of the Circuit Group
For an Amino Acid
(Angle Bending Connections)**

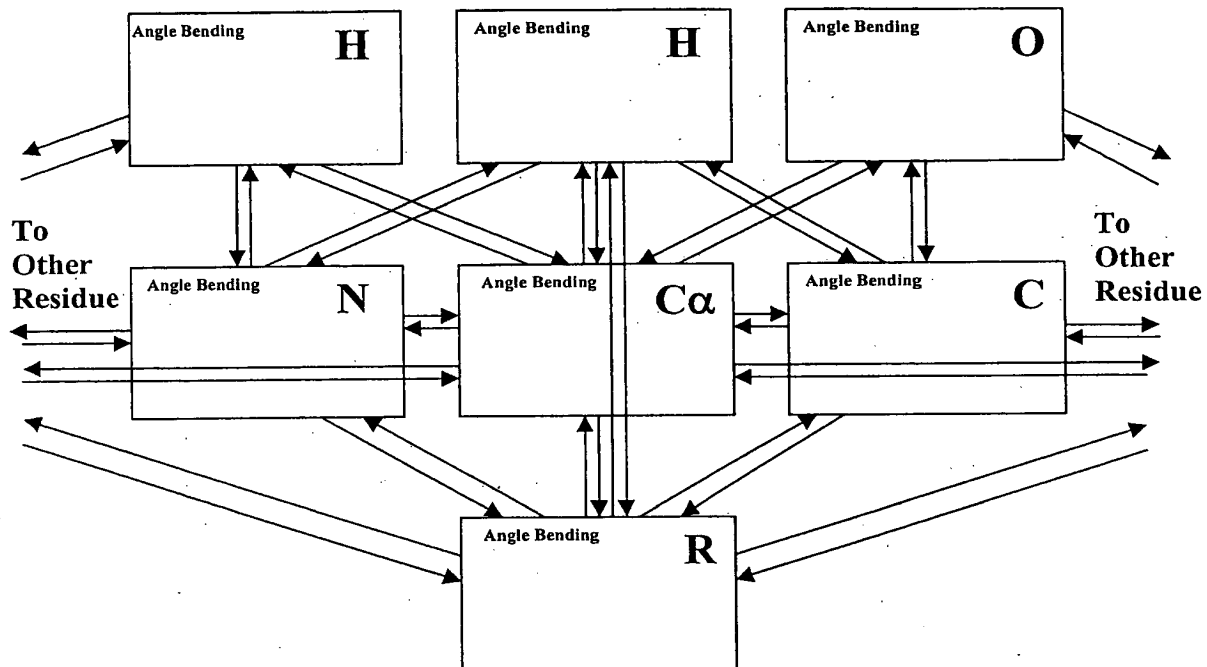


Figure 14

**Illustration of the Circuit Group
For an Amino Acid
(Torsion Connections)**

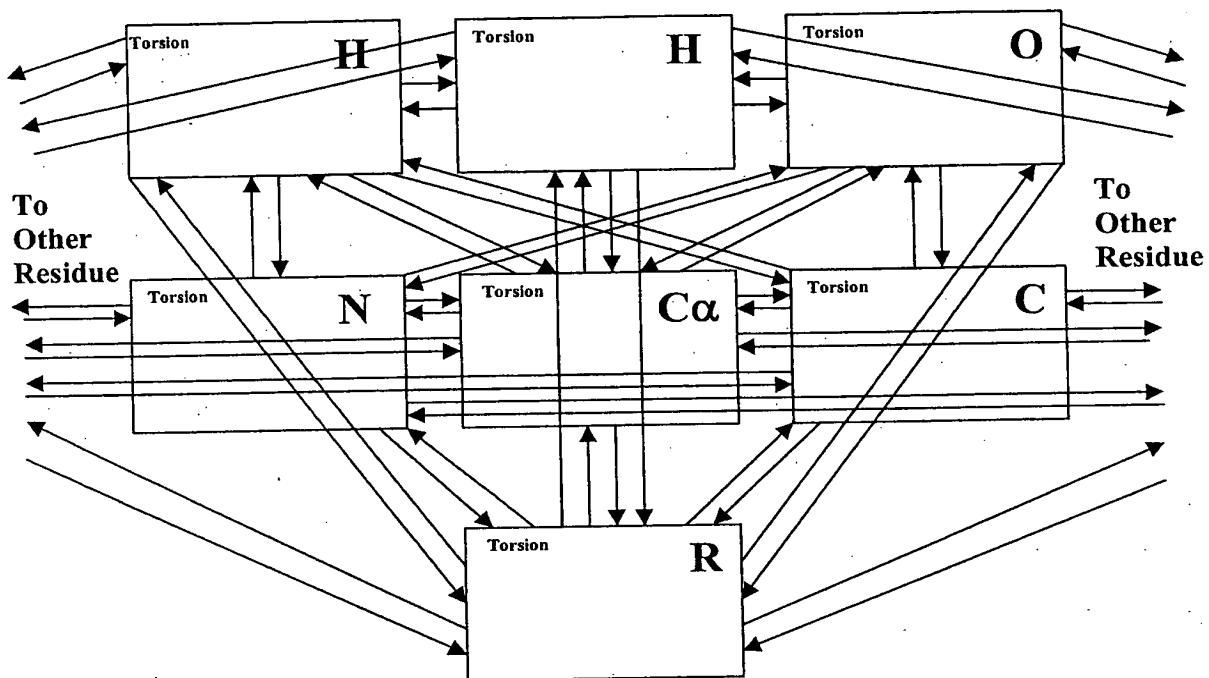


Figure 15

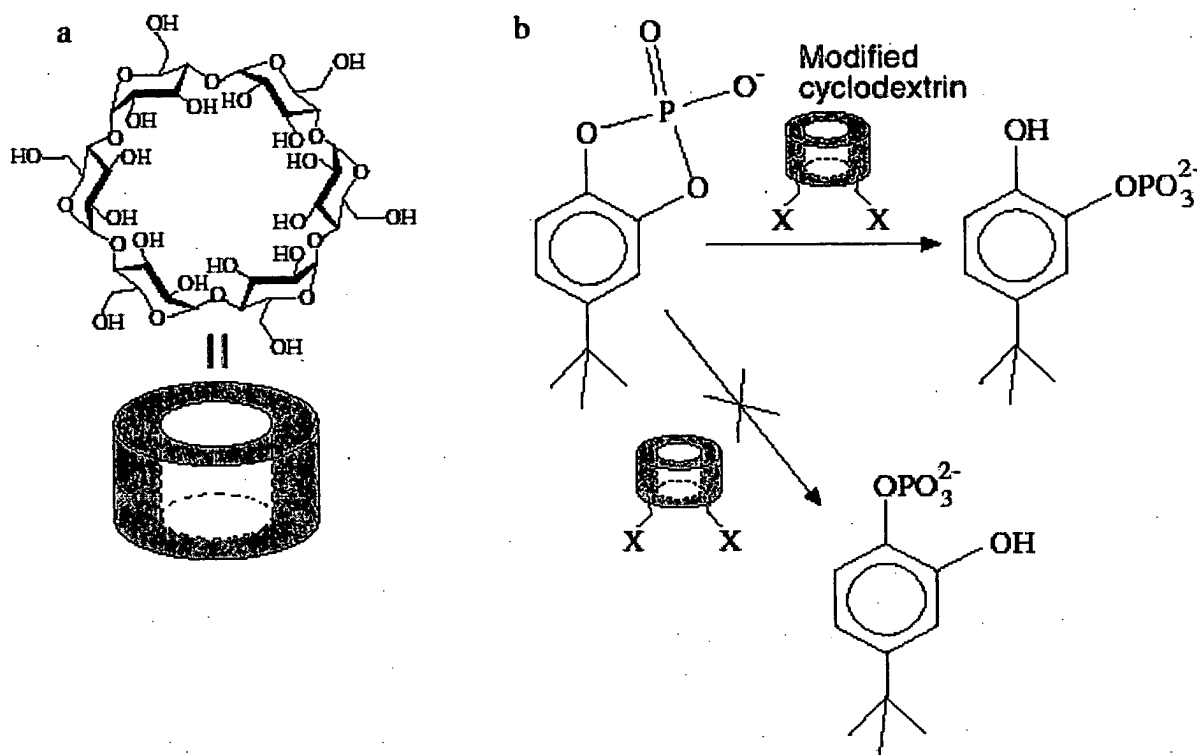


Figure 16

**Illustration of the Circuit Group
For a Sub-Unit in Cyclodextrin
(Bond Stretch Connections)**

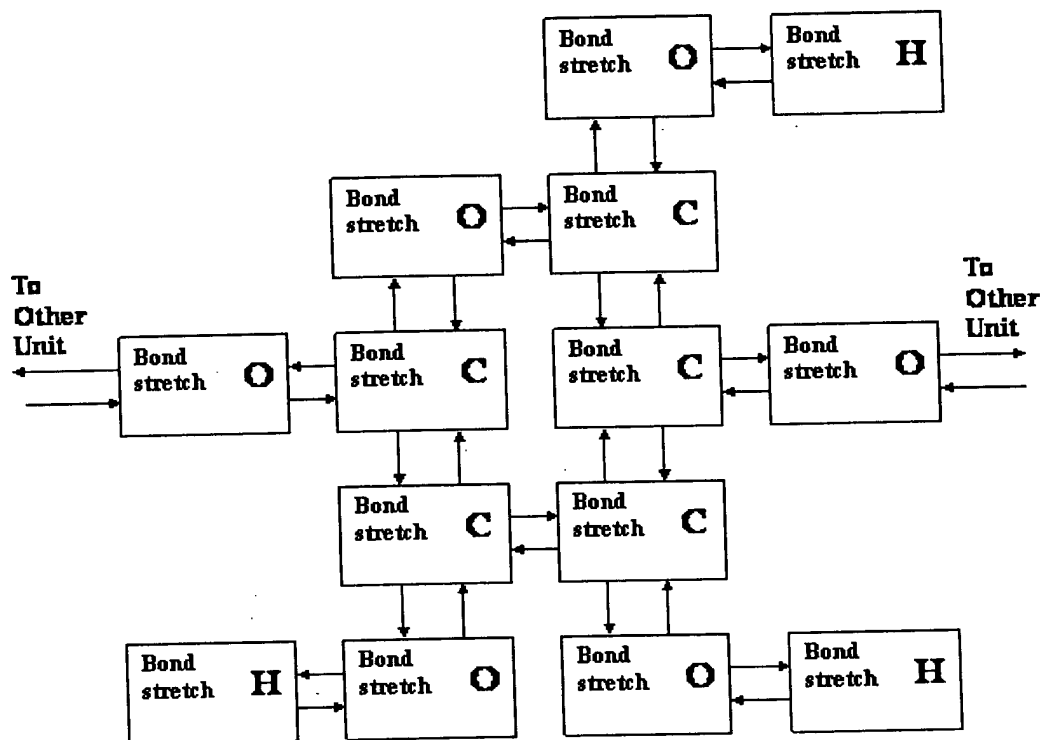


Figure 17

**Illustration of the Circuit Group
For a Sub-Unit in Cyclodextrin
(Angle Bending Connections)**

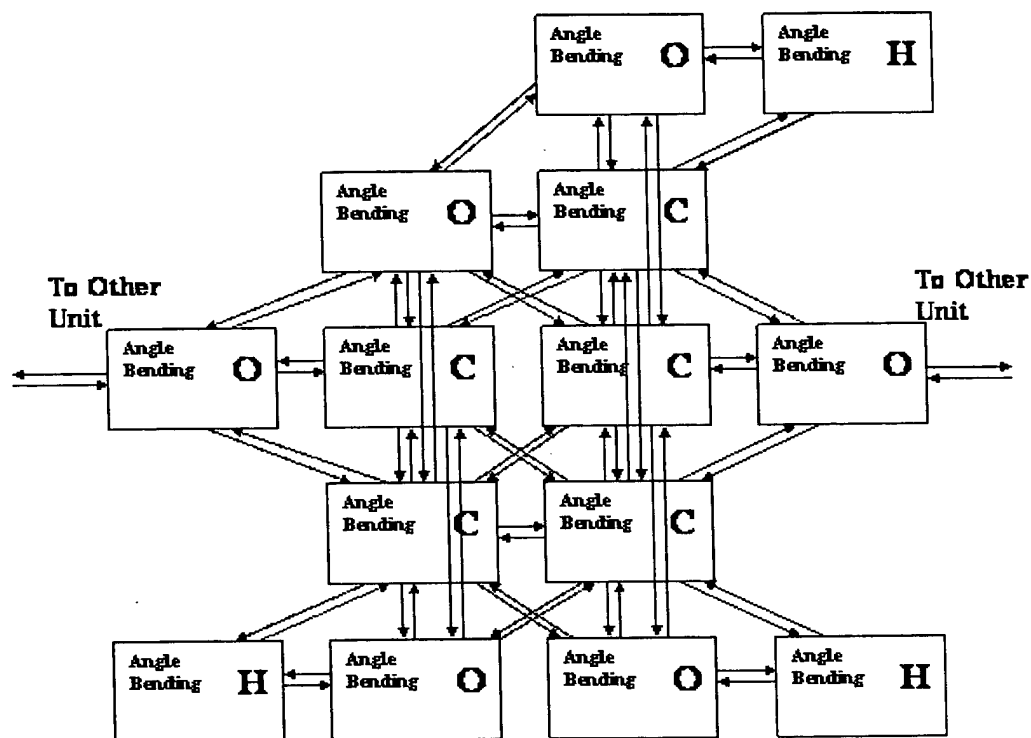


Figure 18

**Illustration of the Circuit Group
For a Sub-Unit in Cyclodextrin
(Angle Bending Connections)**

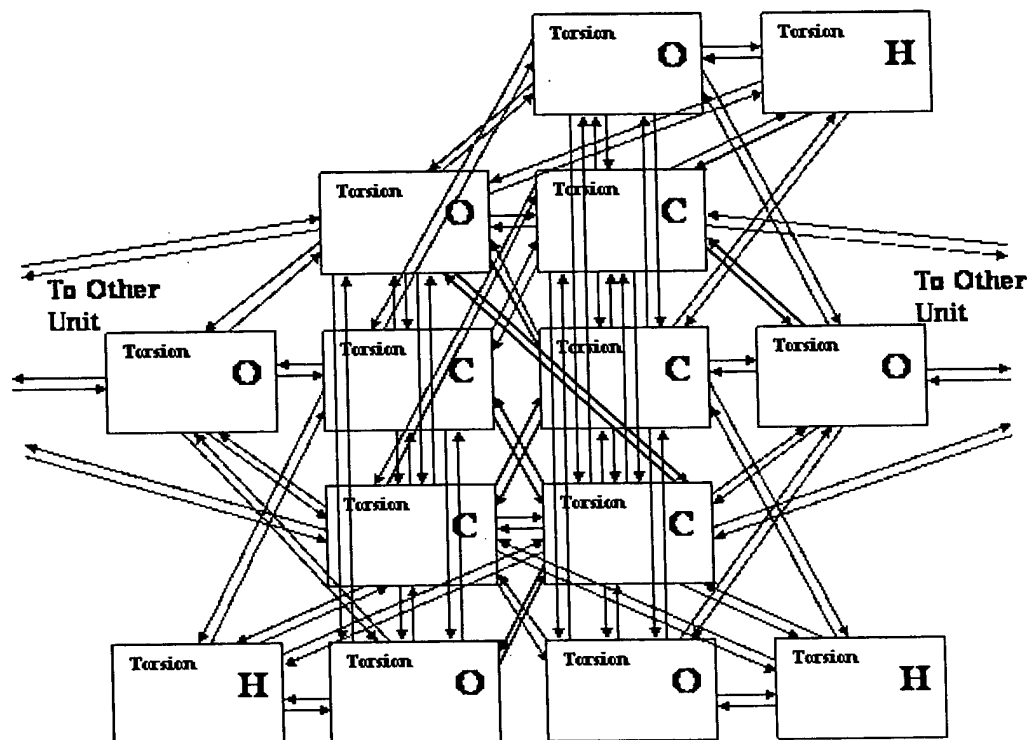


Figure 19

Bond Stretch X Unit

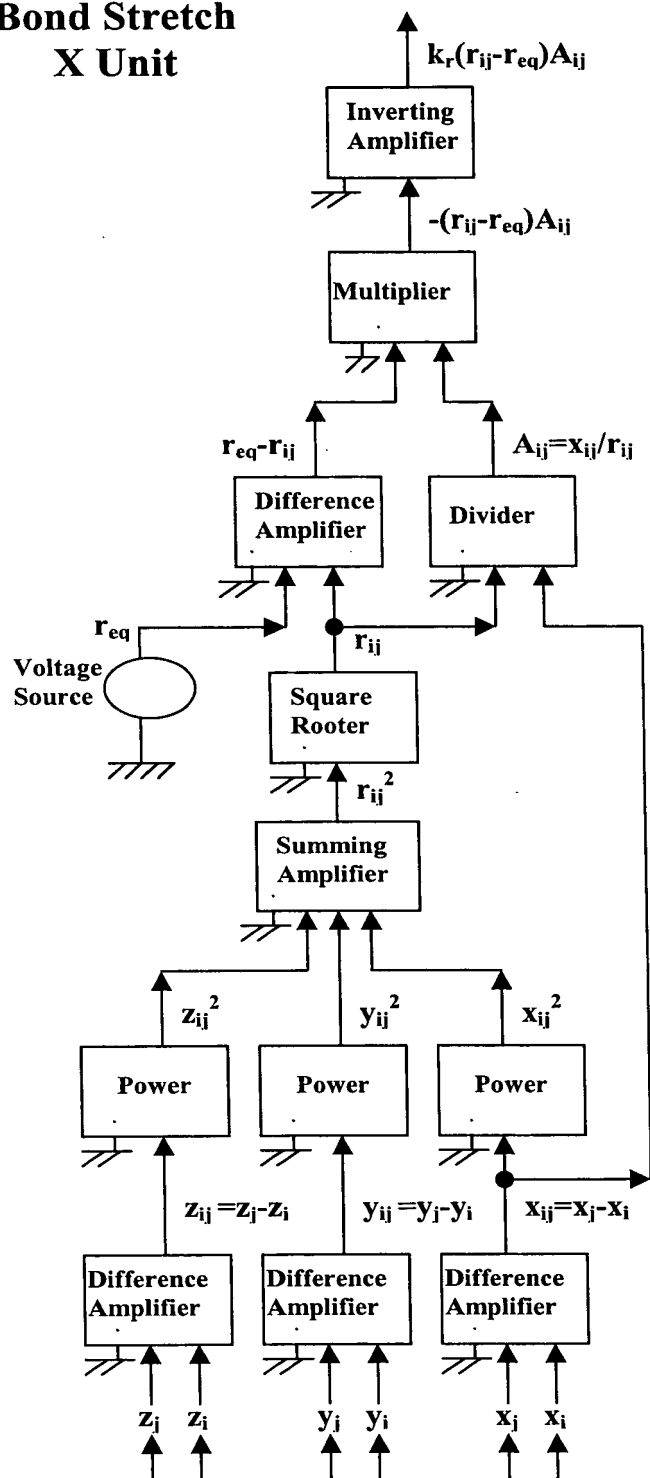


Figure 20

Bond Stretch Y Unit

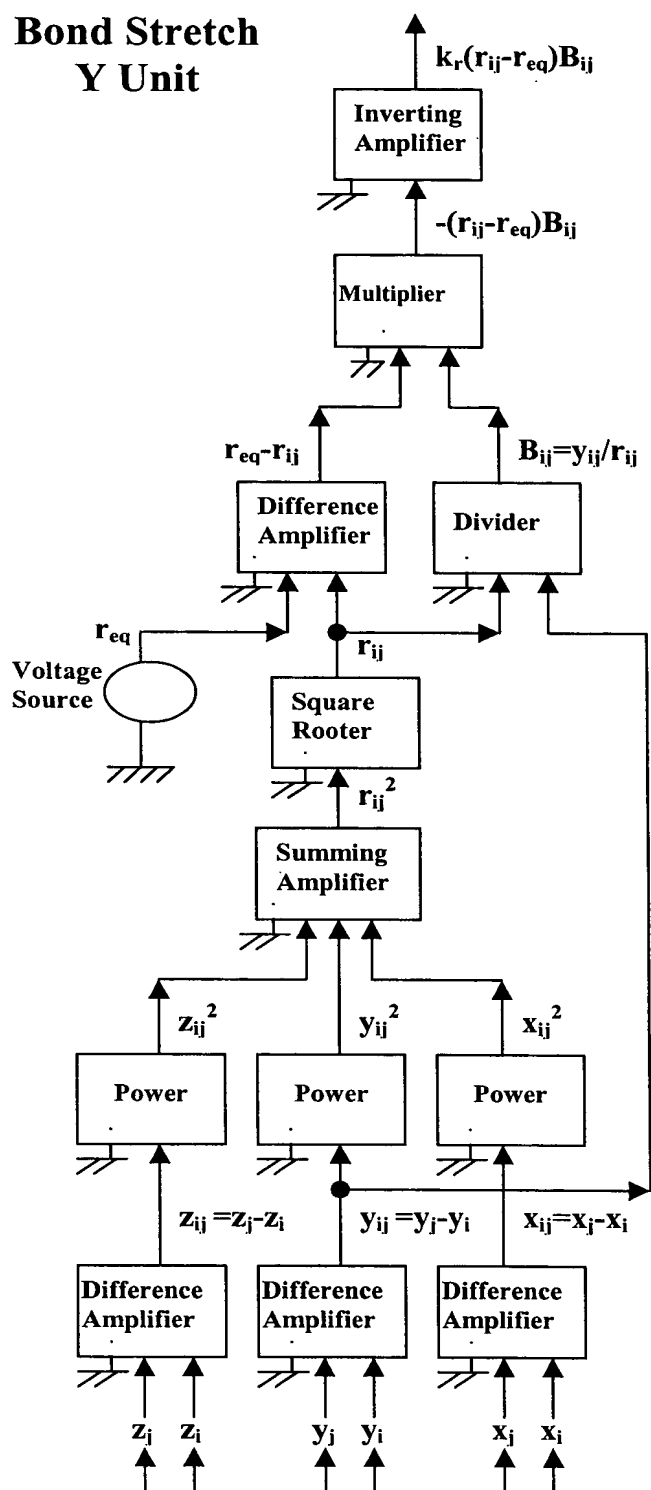


Figure 21

Bond Stretch Z Unit

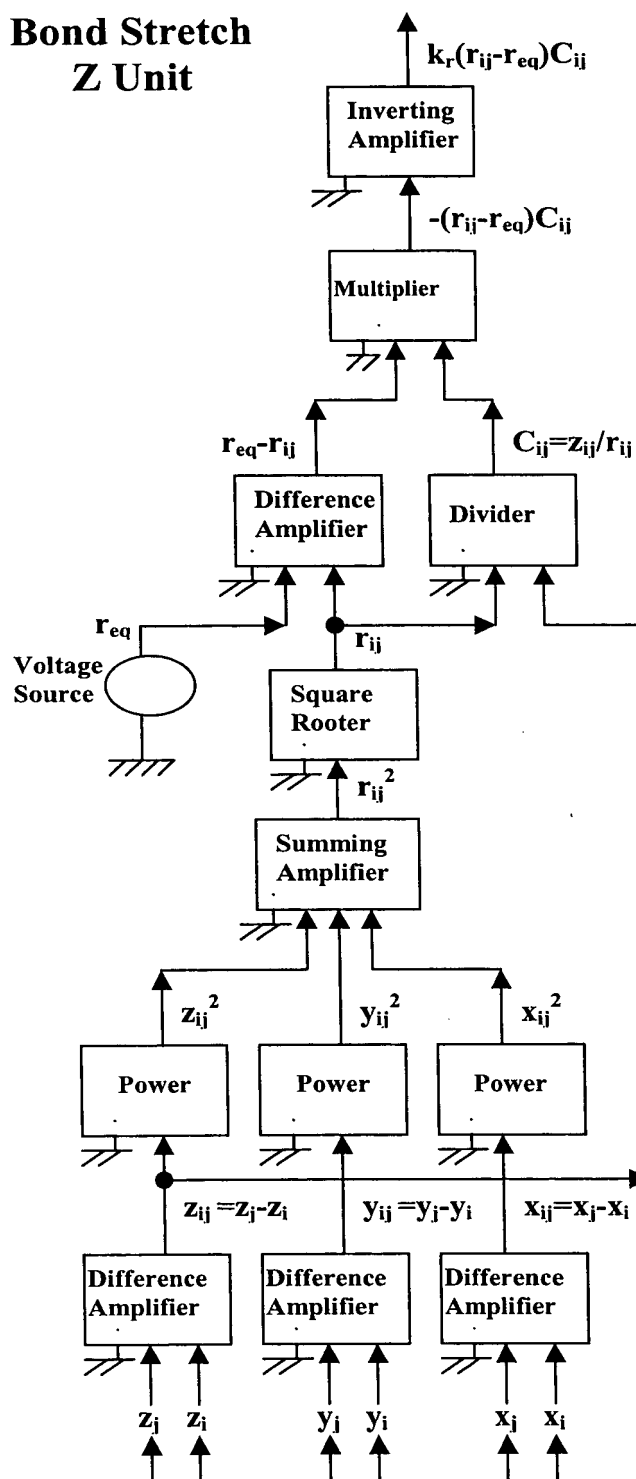


Figure 22

Angle Bending
X Unit
Type A

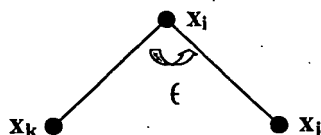
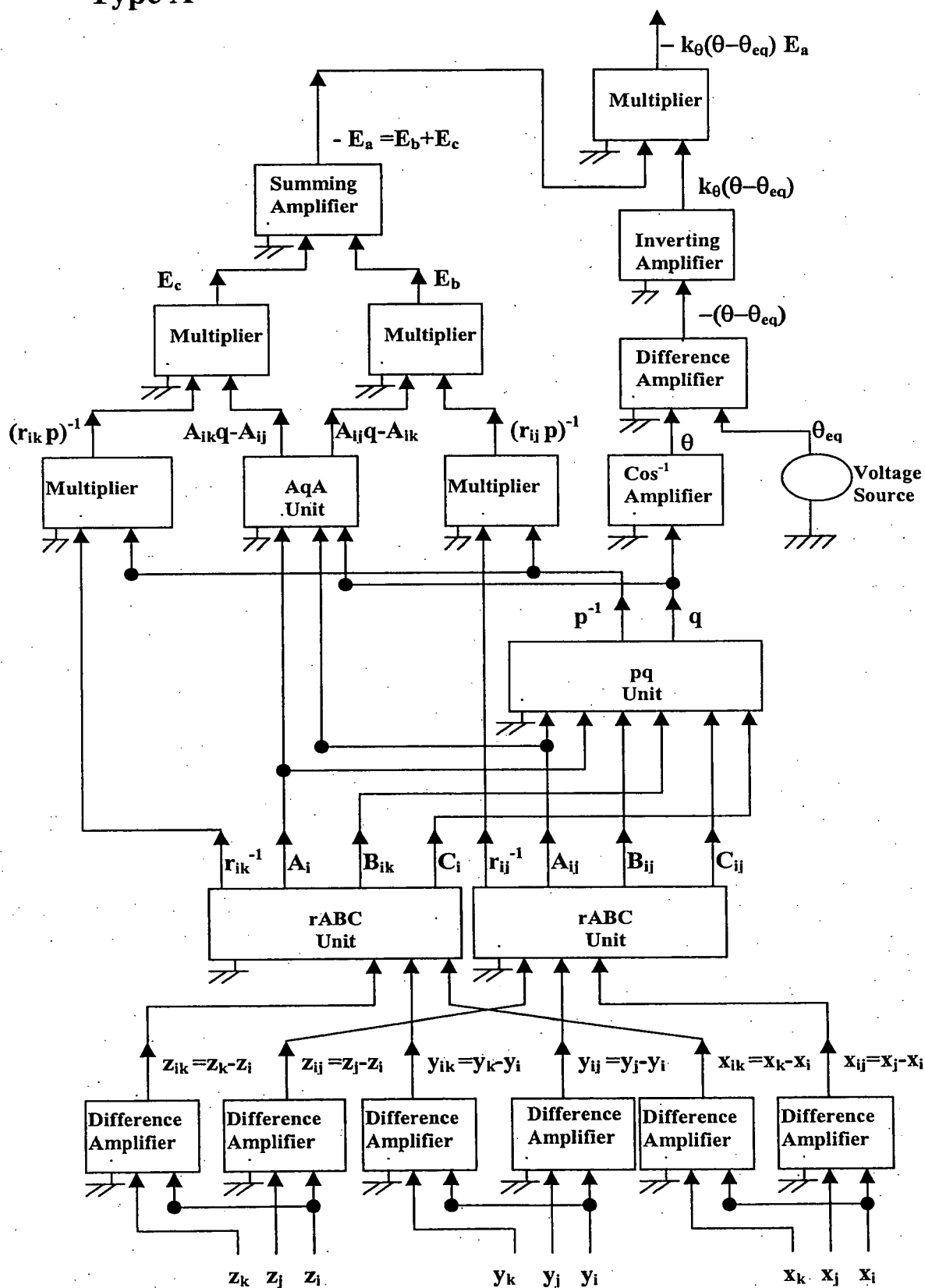


Figure 23



Angle Bending
X Unit
Type B

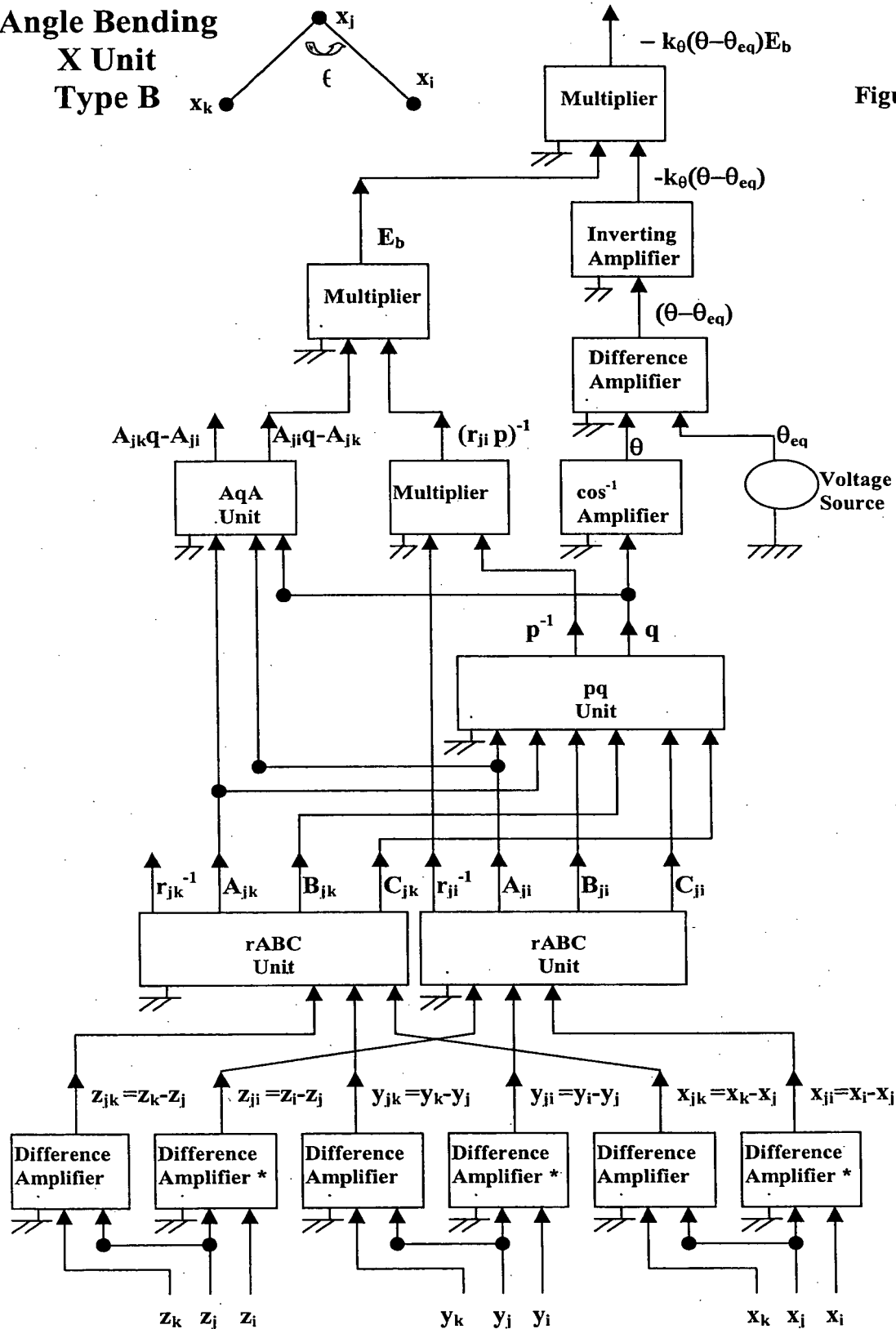


Figure 24

Angle Bending
Y Unit
Type A

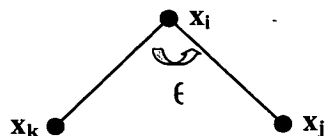


Figure 25

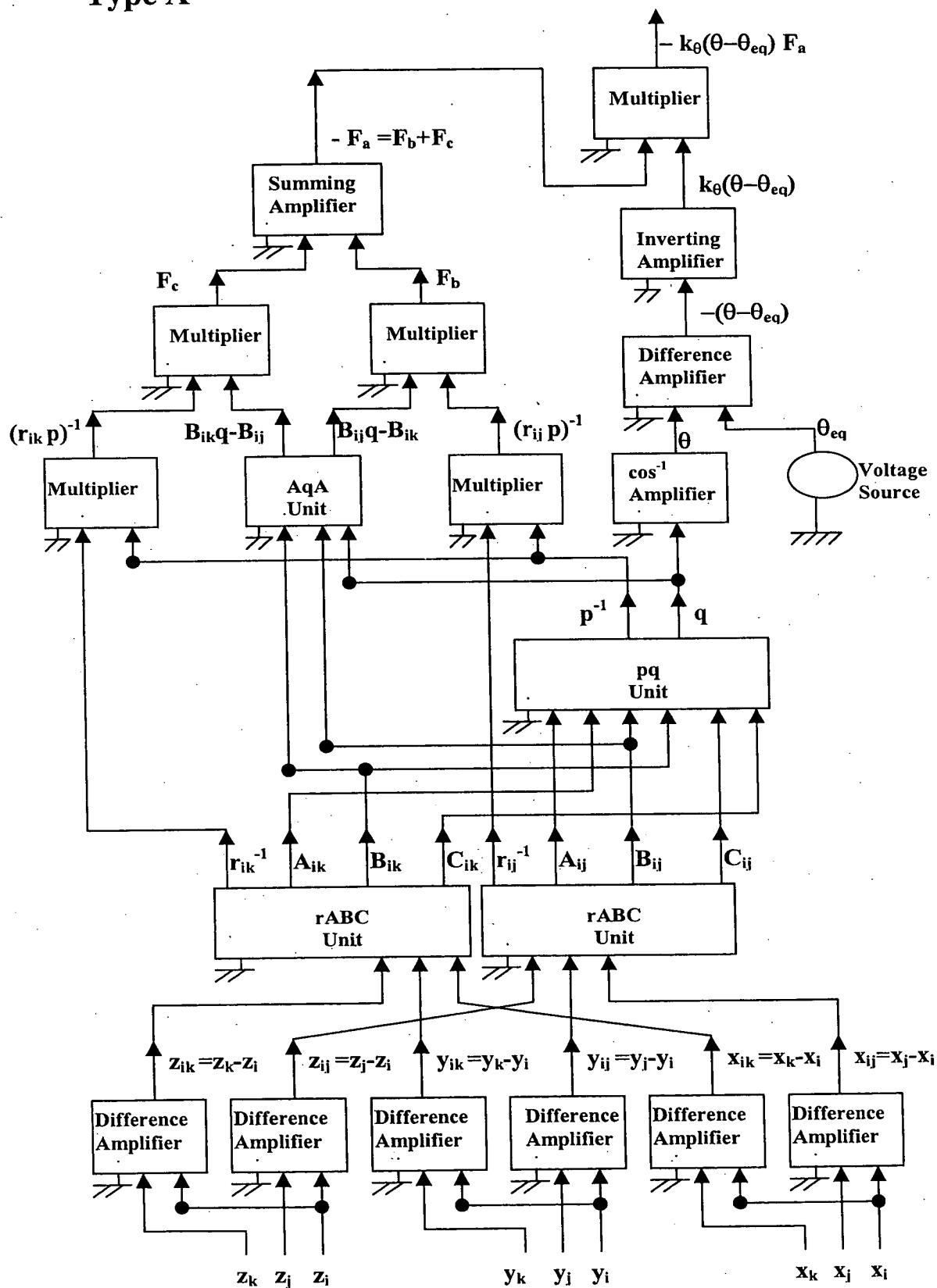
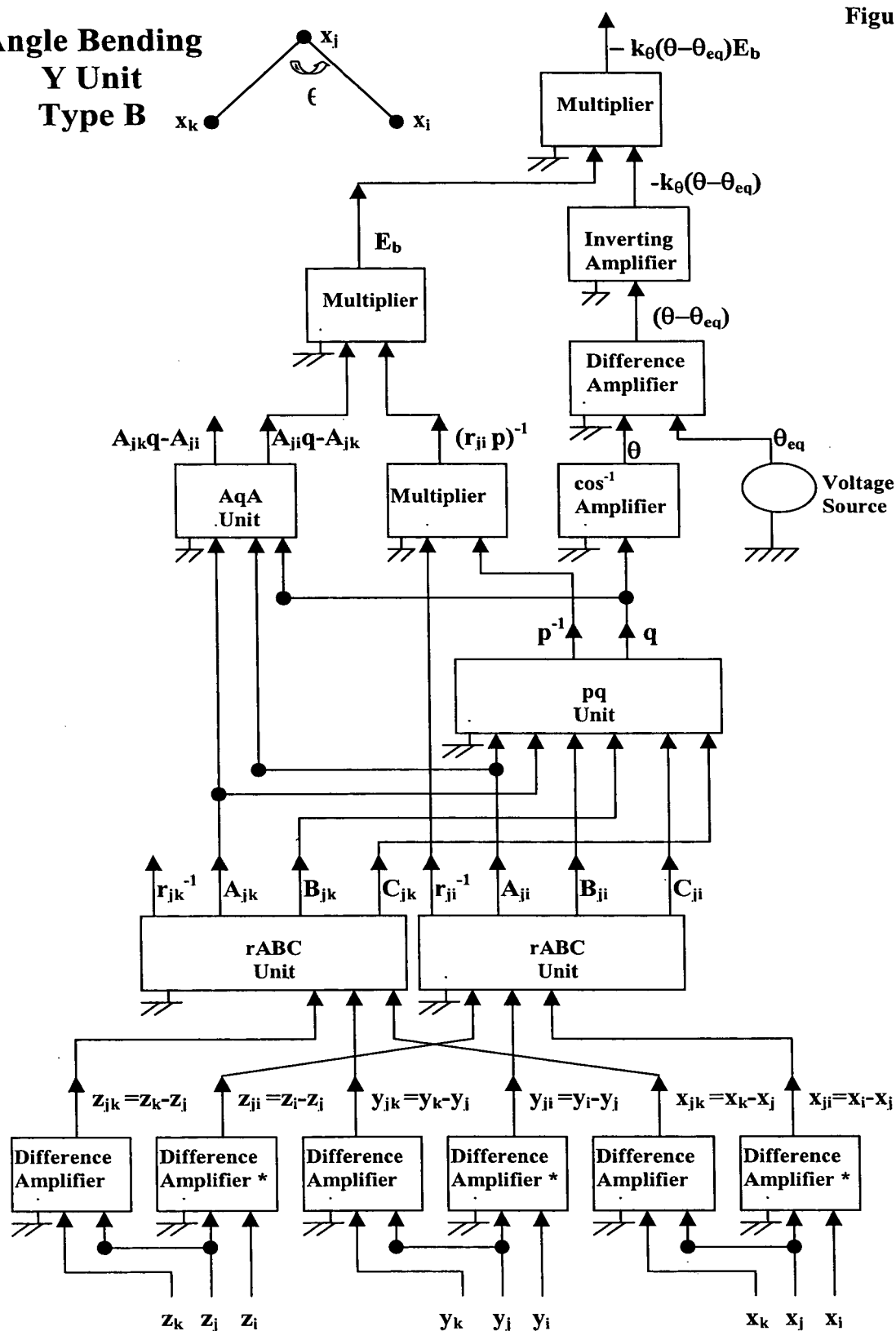


Figure 26

Angle Bending
Y Unit
Type B



Angle Bending
Z Unit
Type A

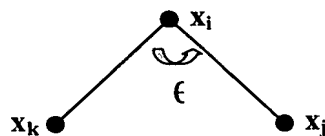


Figure 27

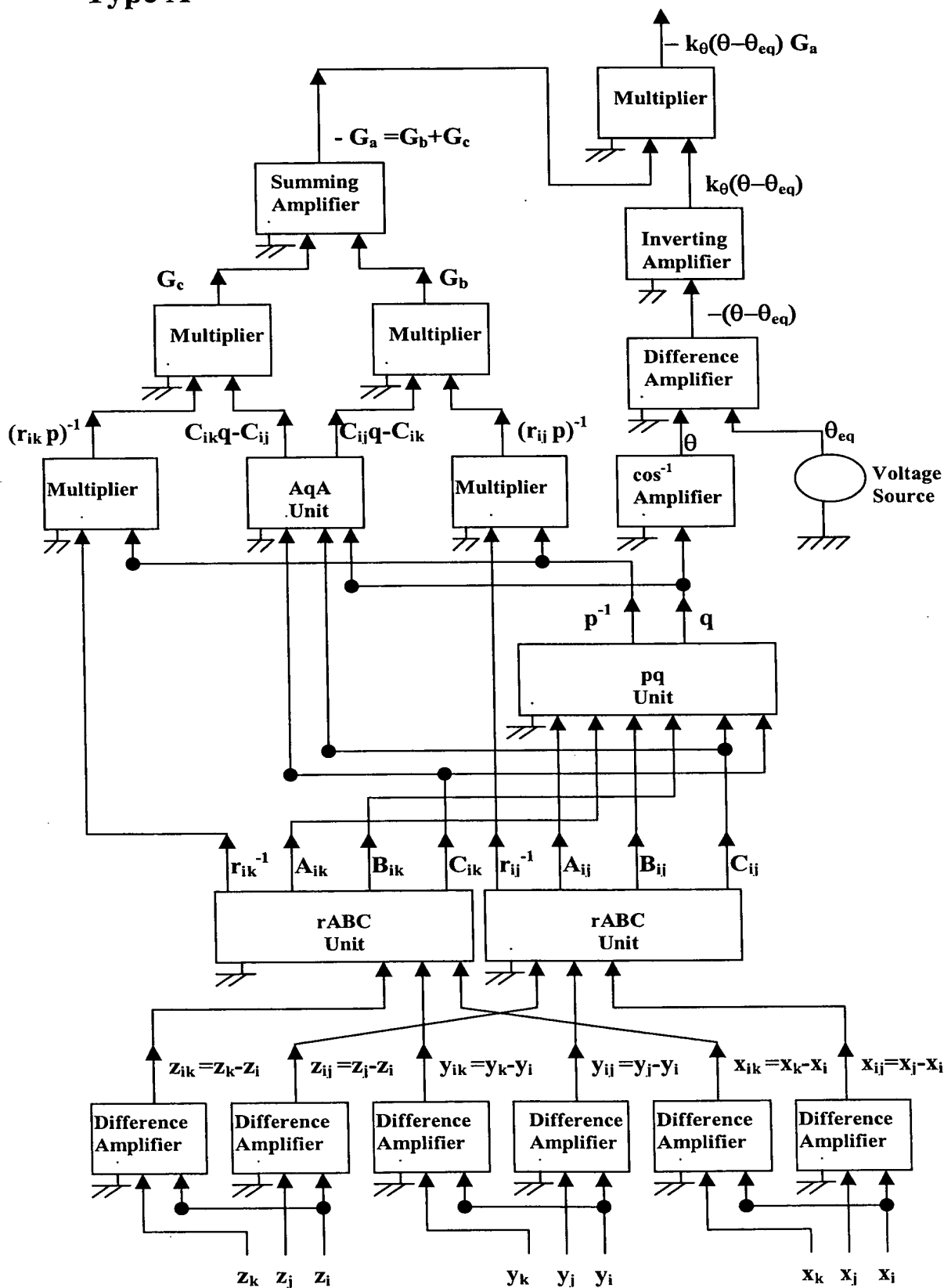
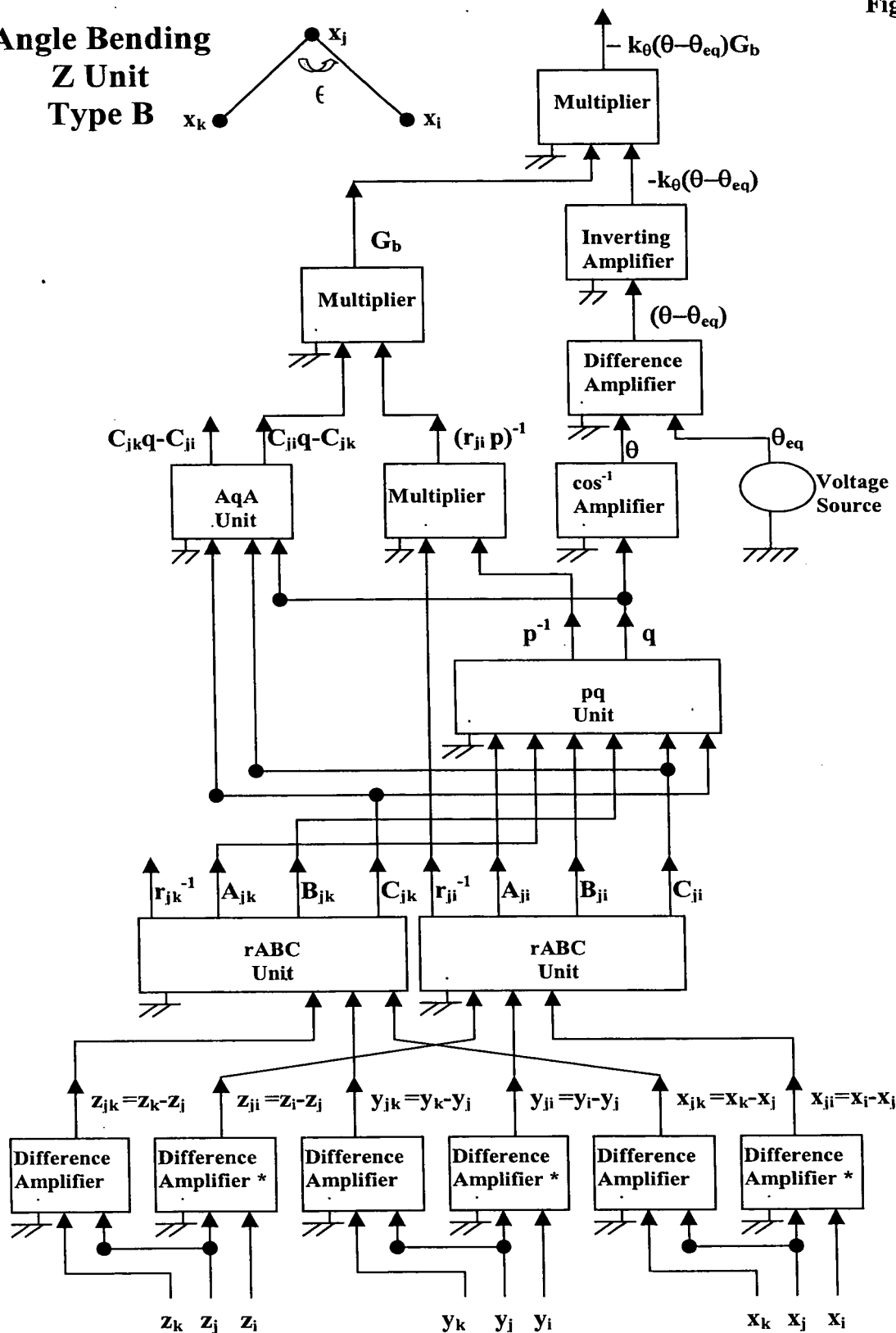


Figure 28

Angle Bending
Z Unit
Type B



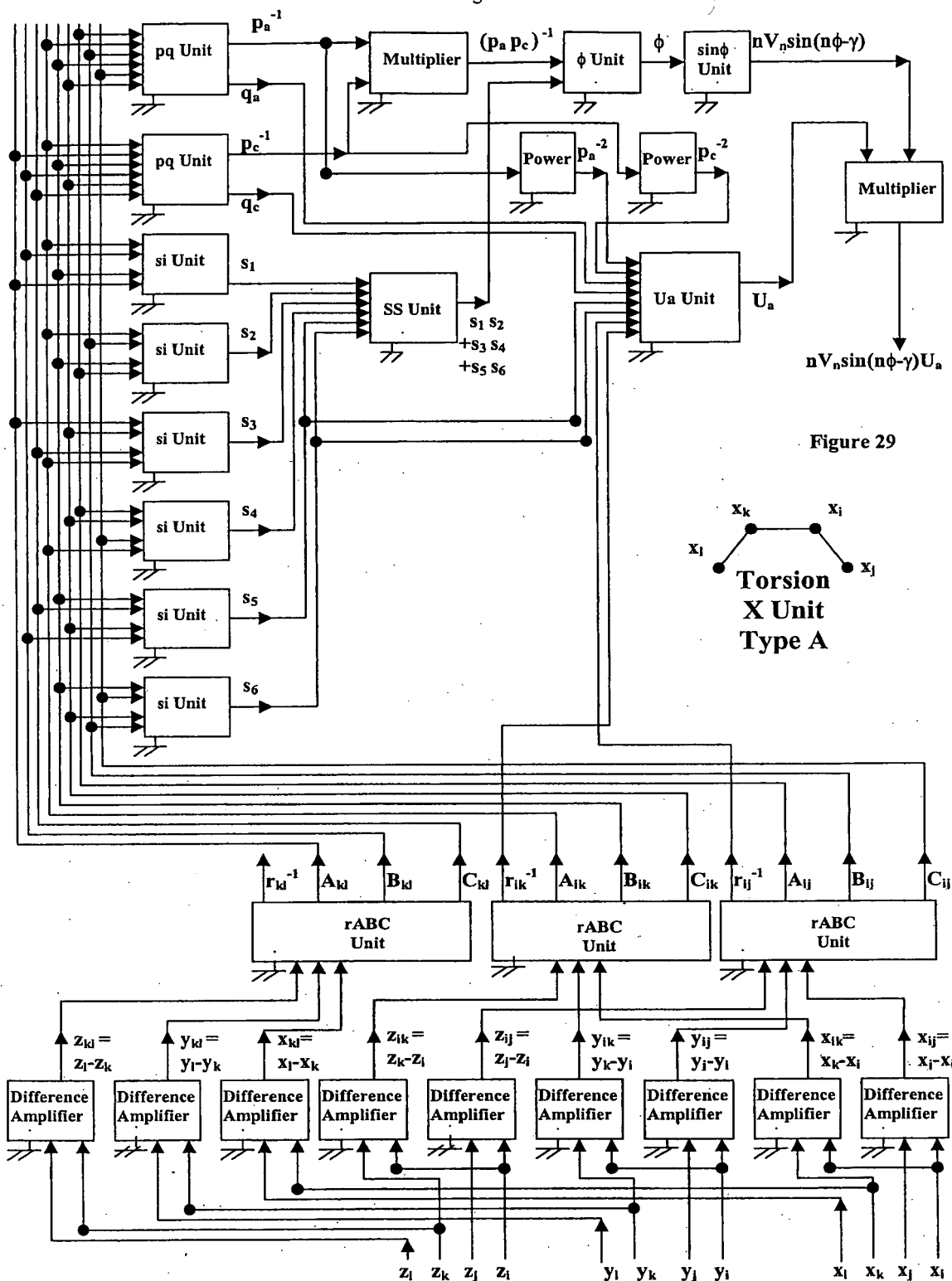
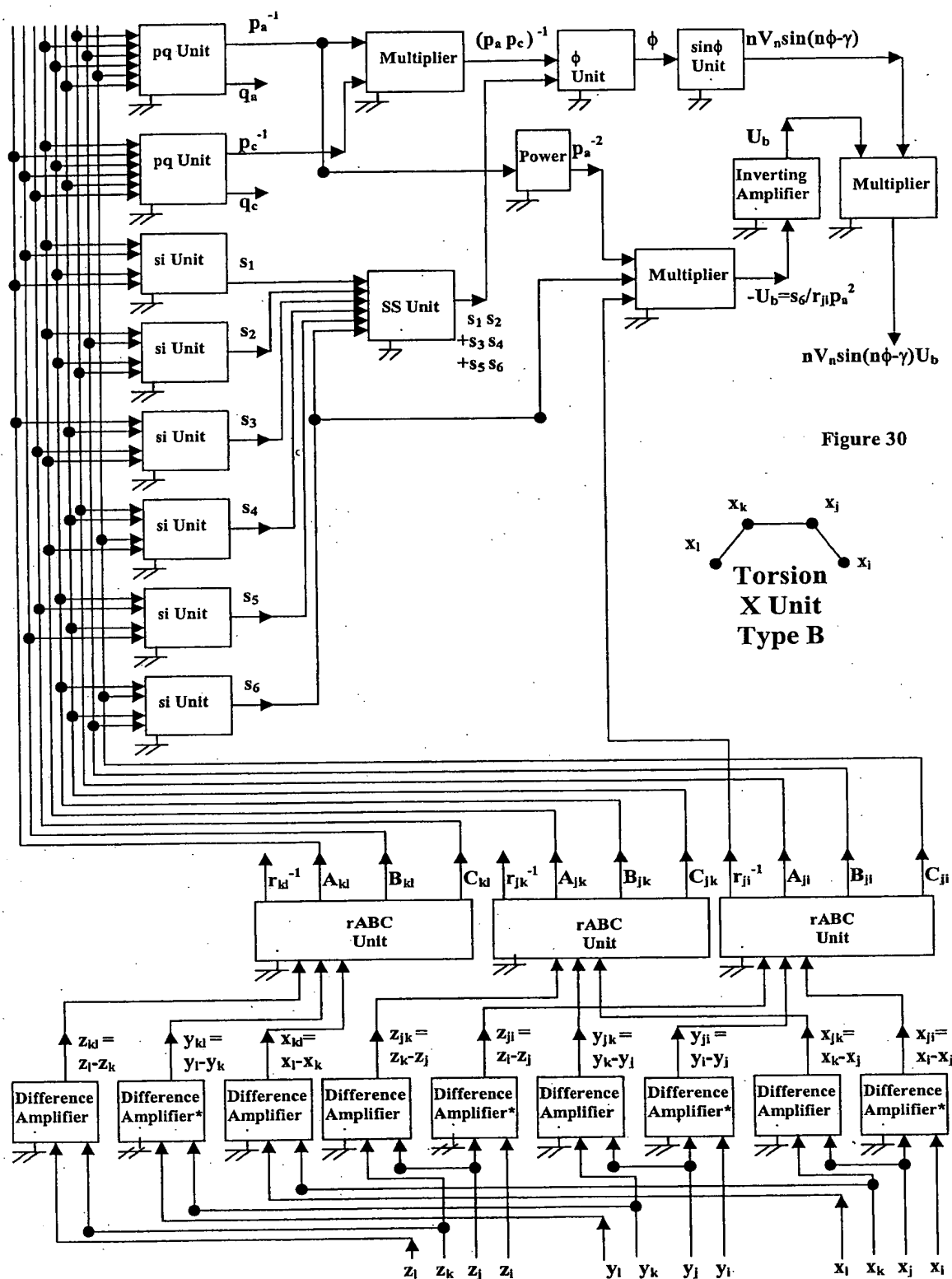
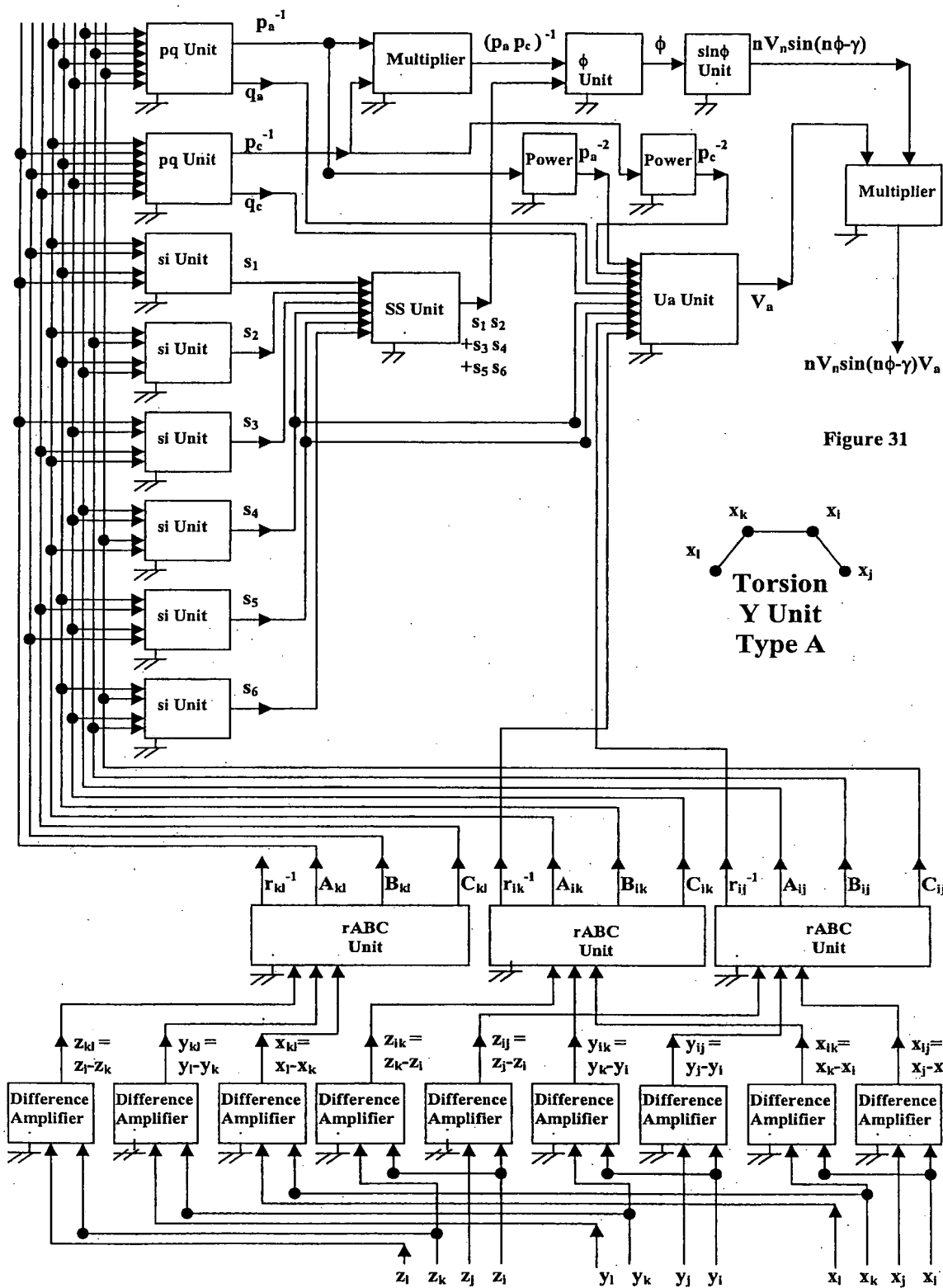


Figure 29





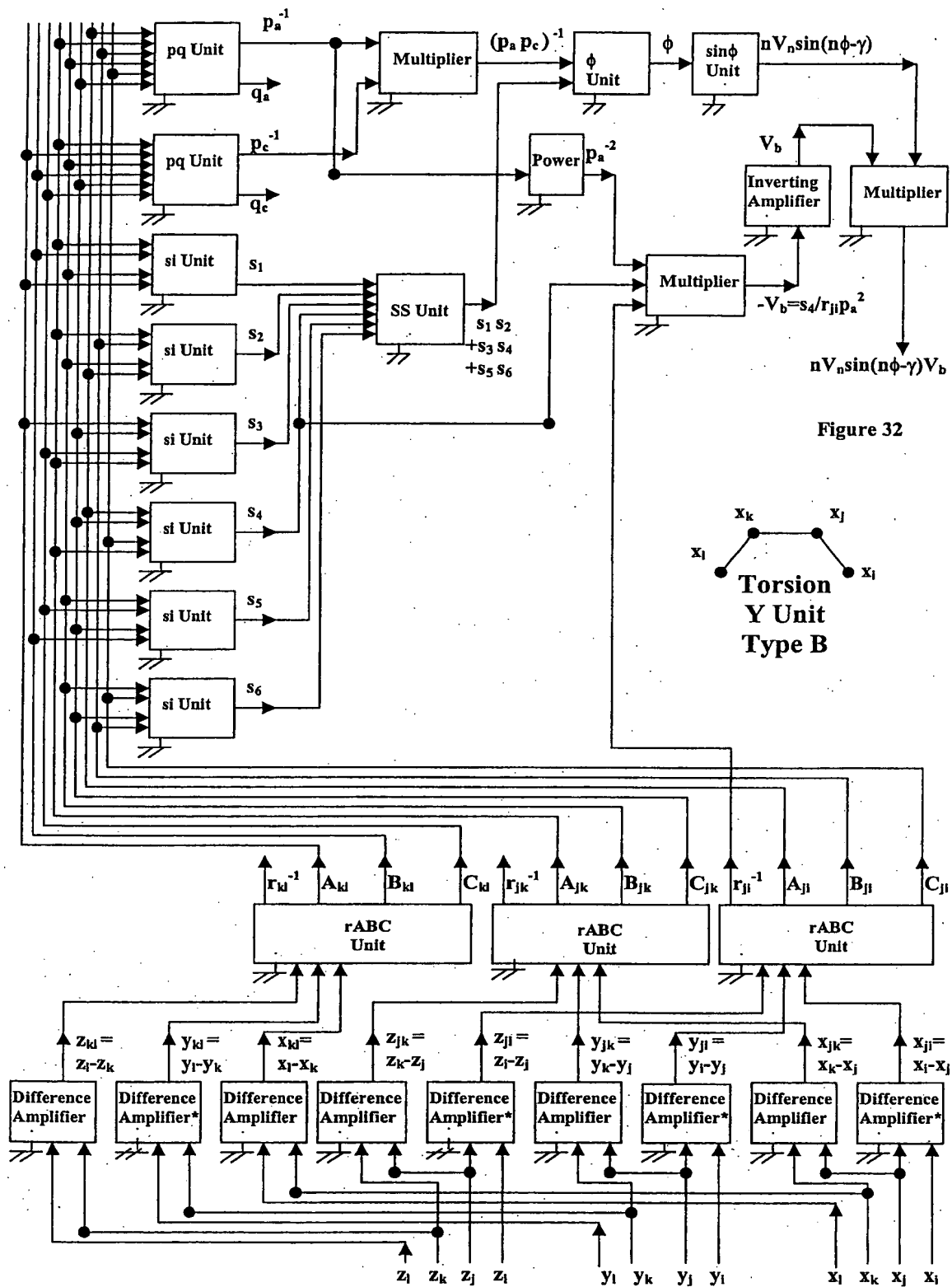


Figure 32



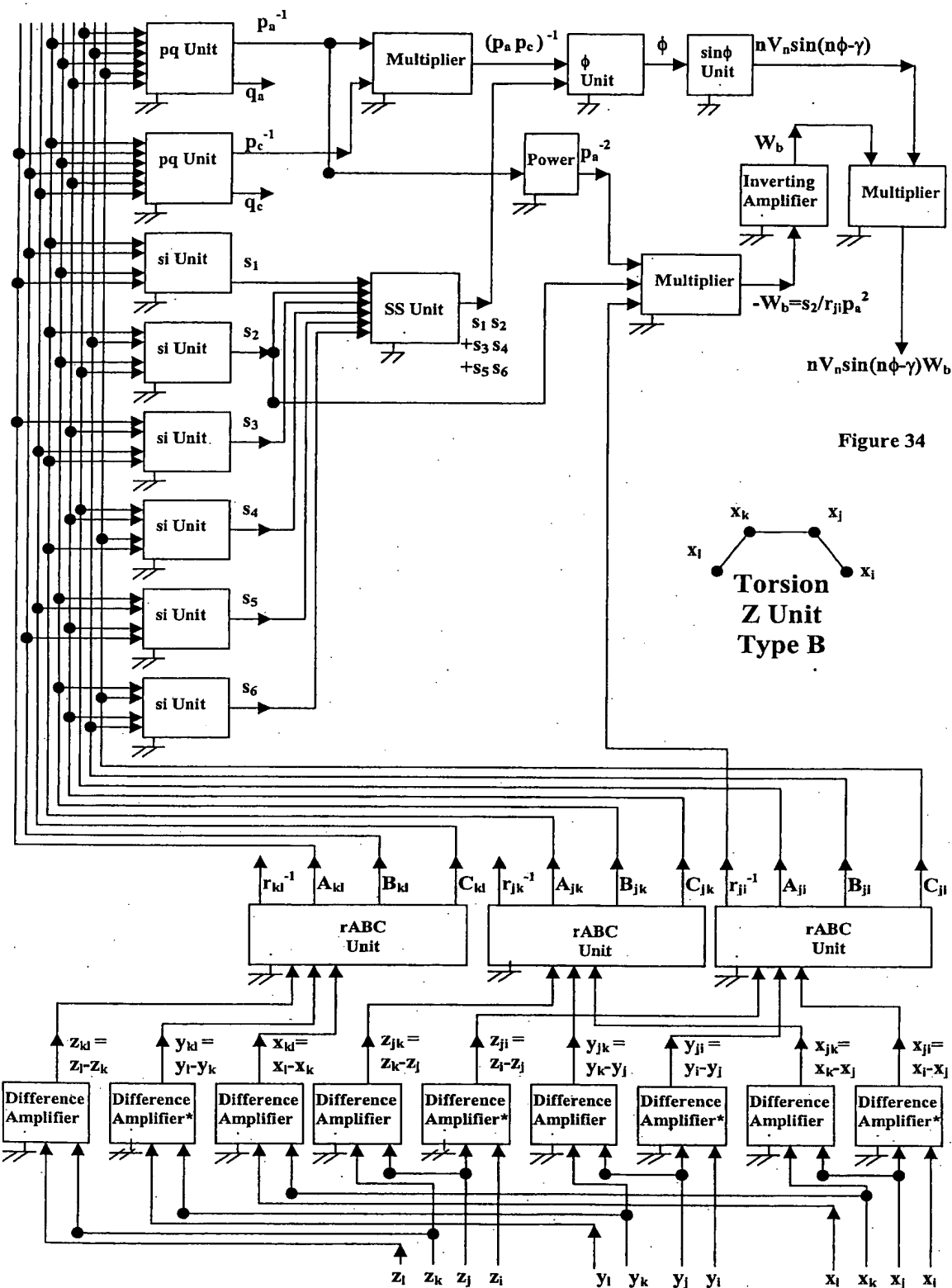


Figure 34

Non-bonded X Unit

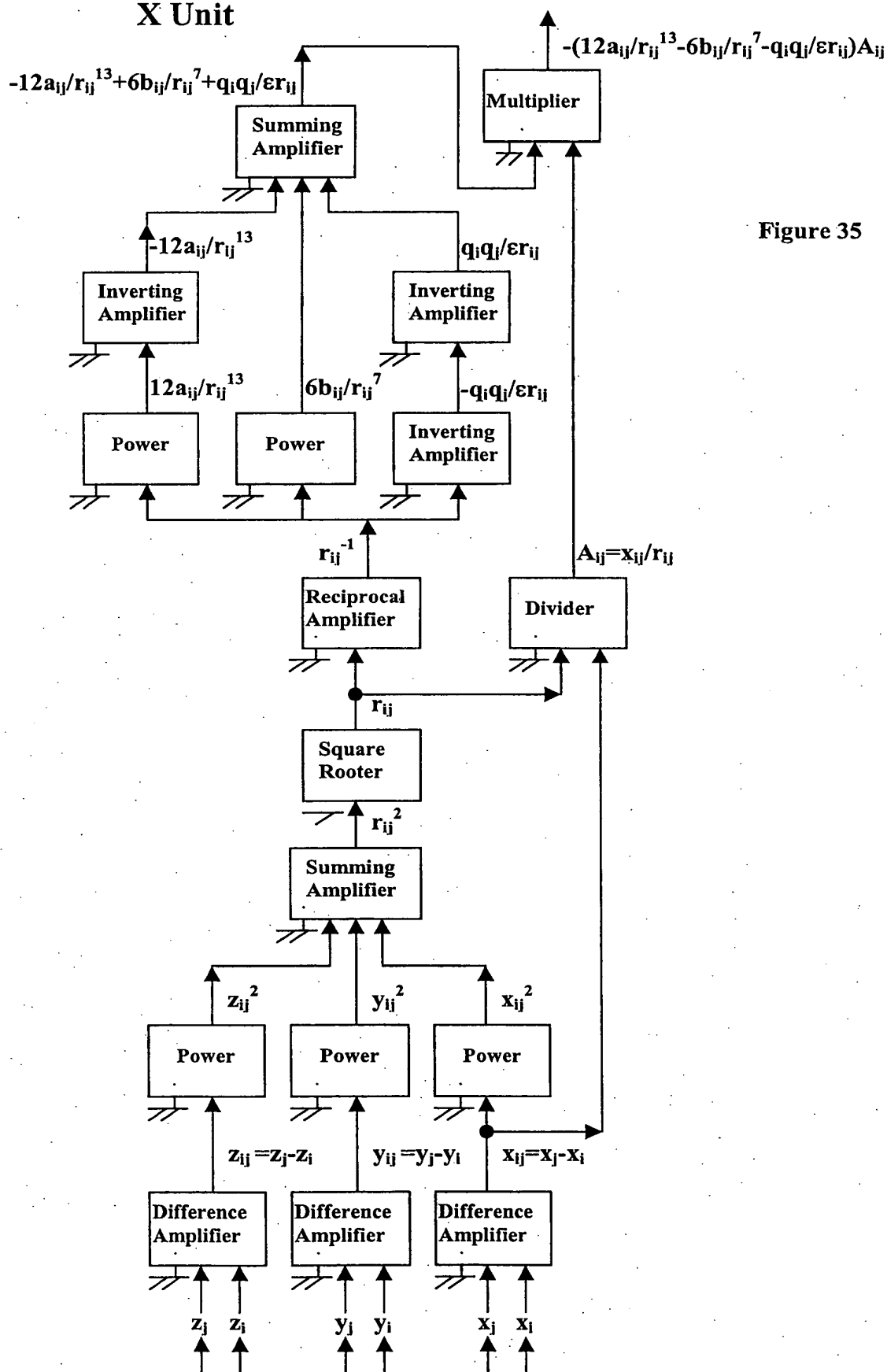


Figure 35

Non-bonded Y Unit

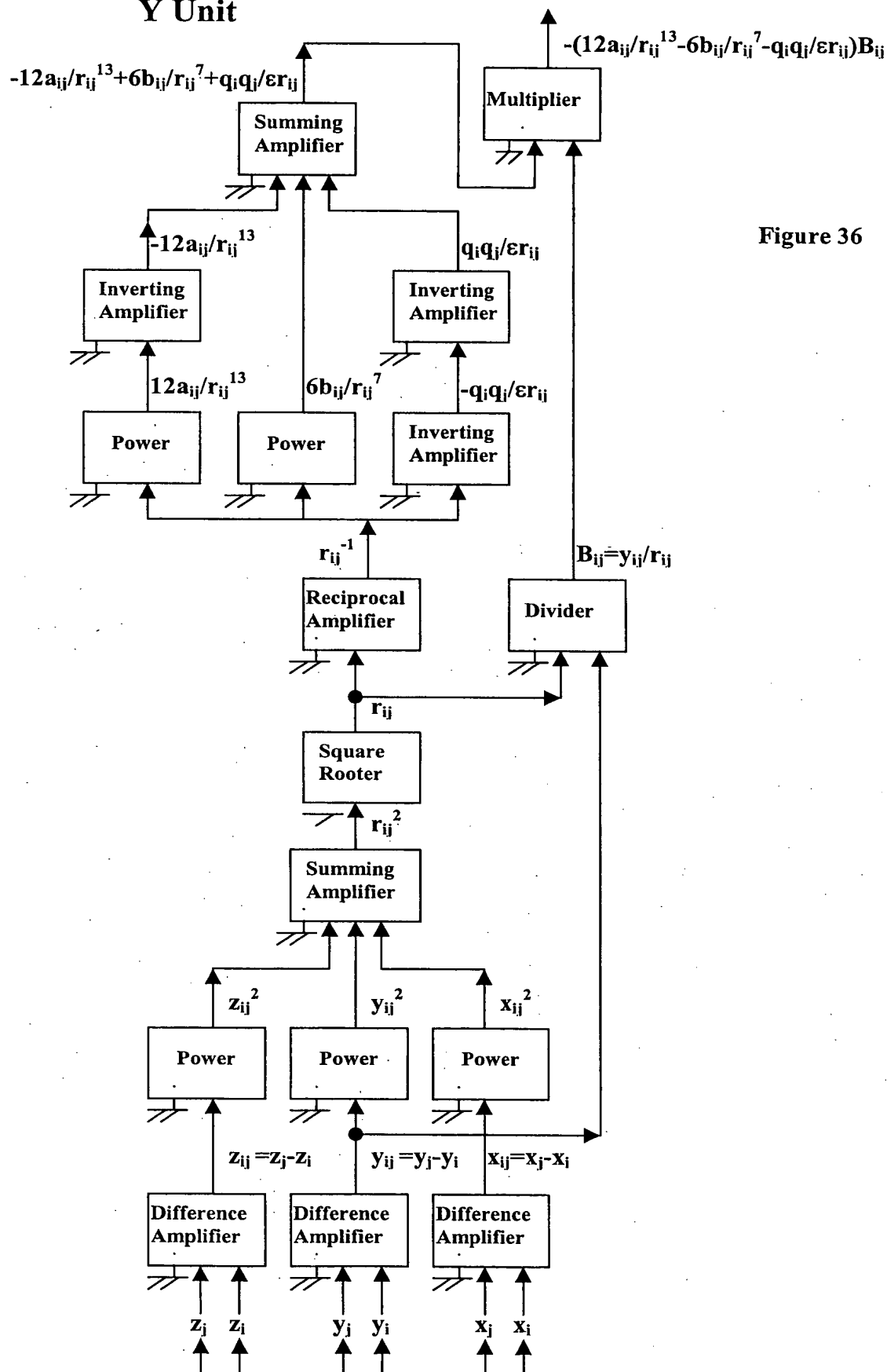


Figure 36

Non-bonded Z Unit

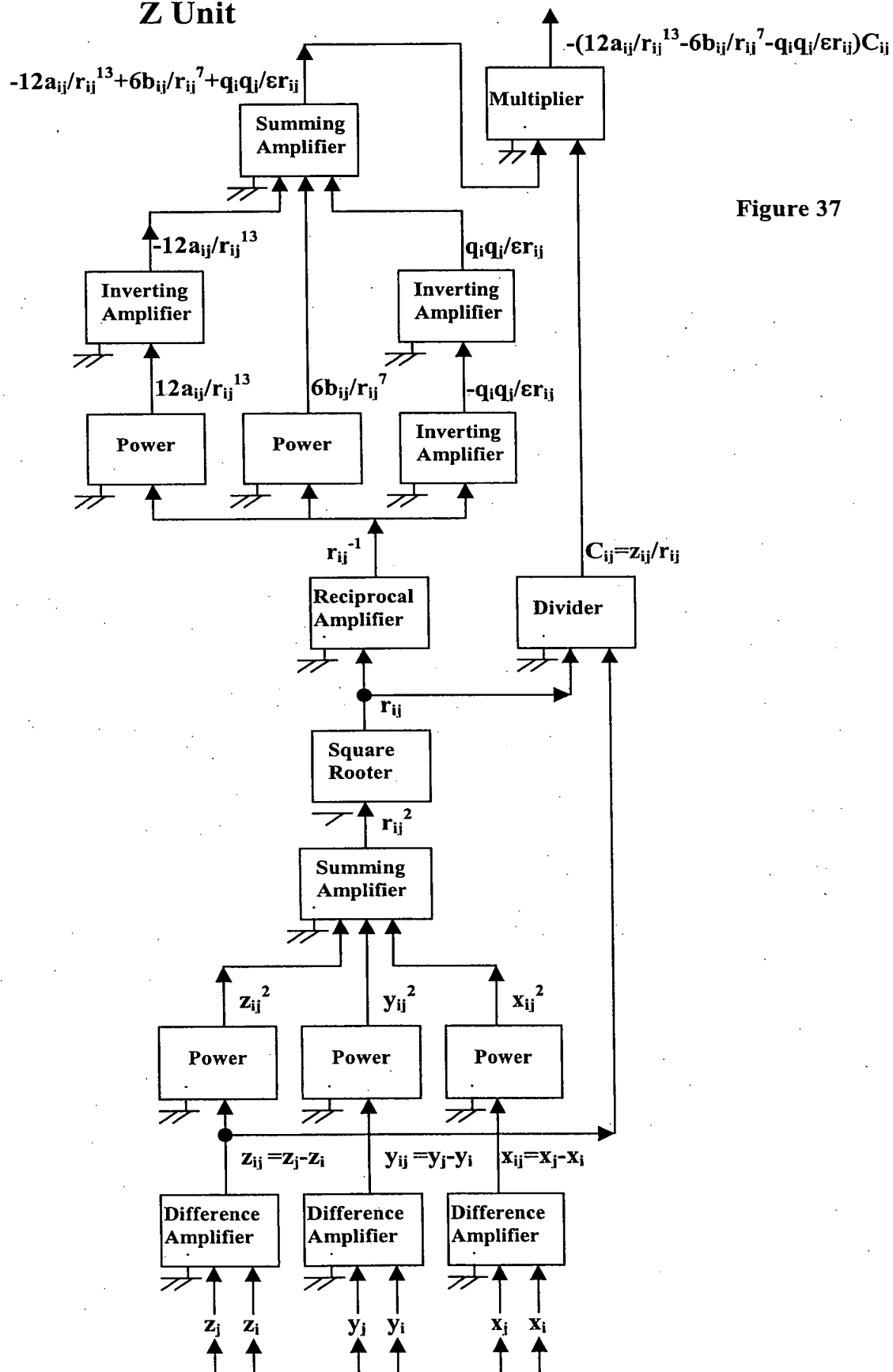


Figure 37

H-bond
X Unit

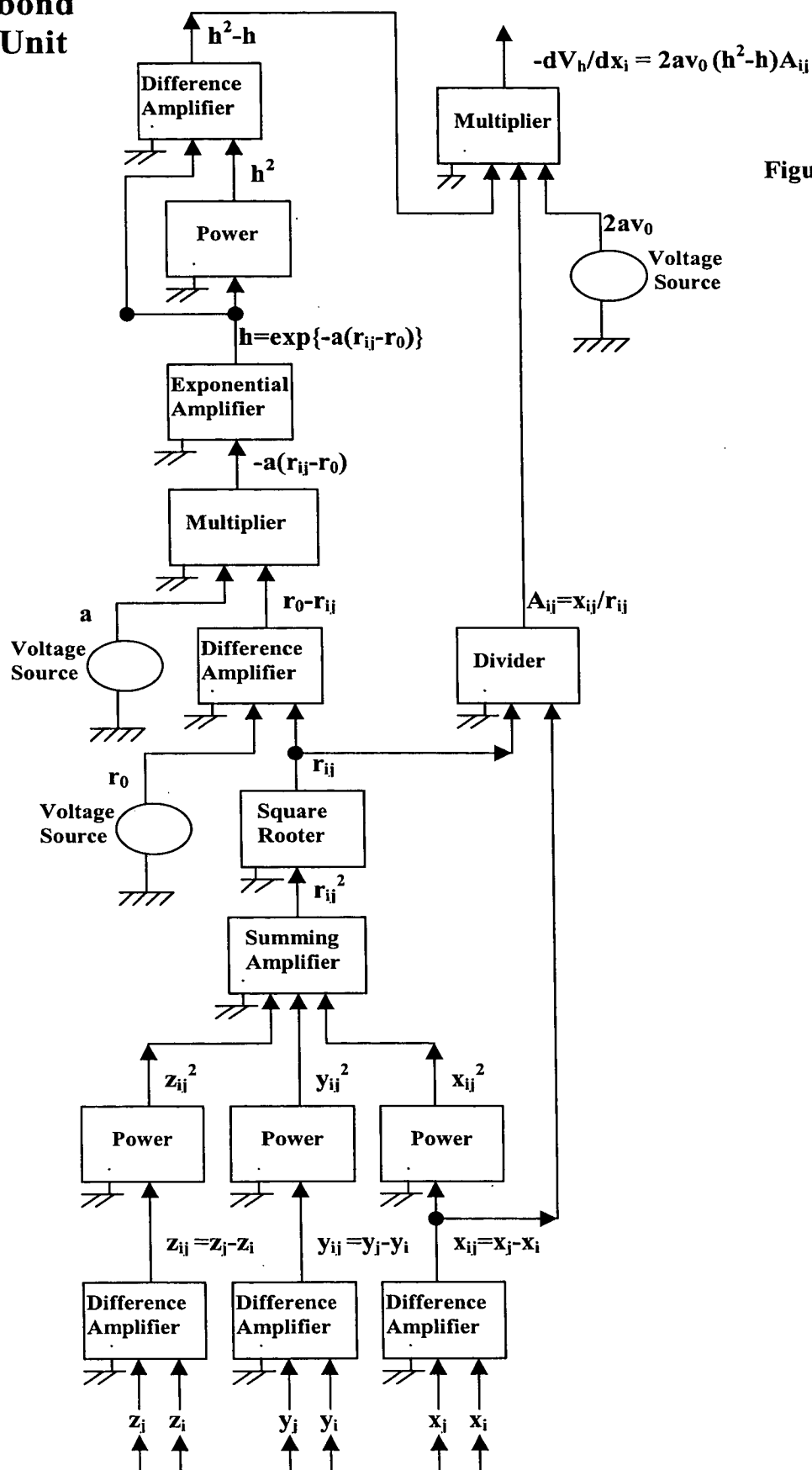


Figure 38

H-bond Y Unit

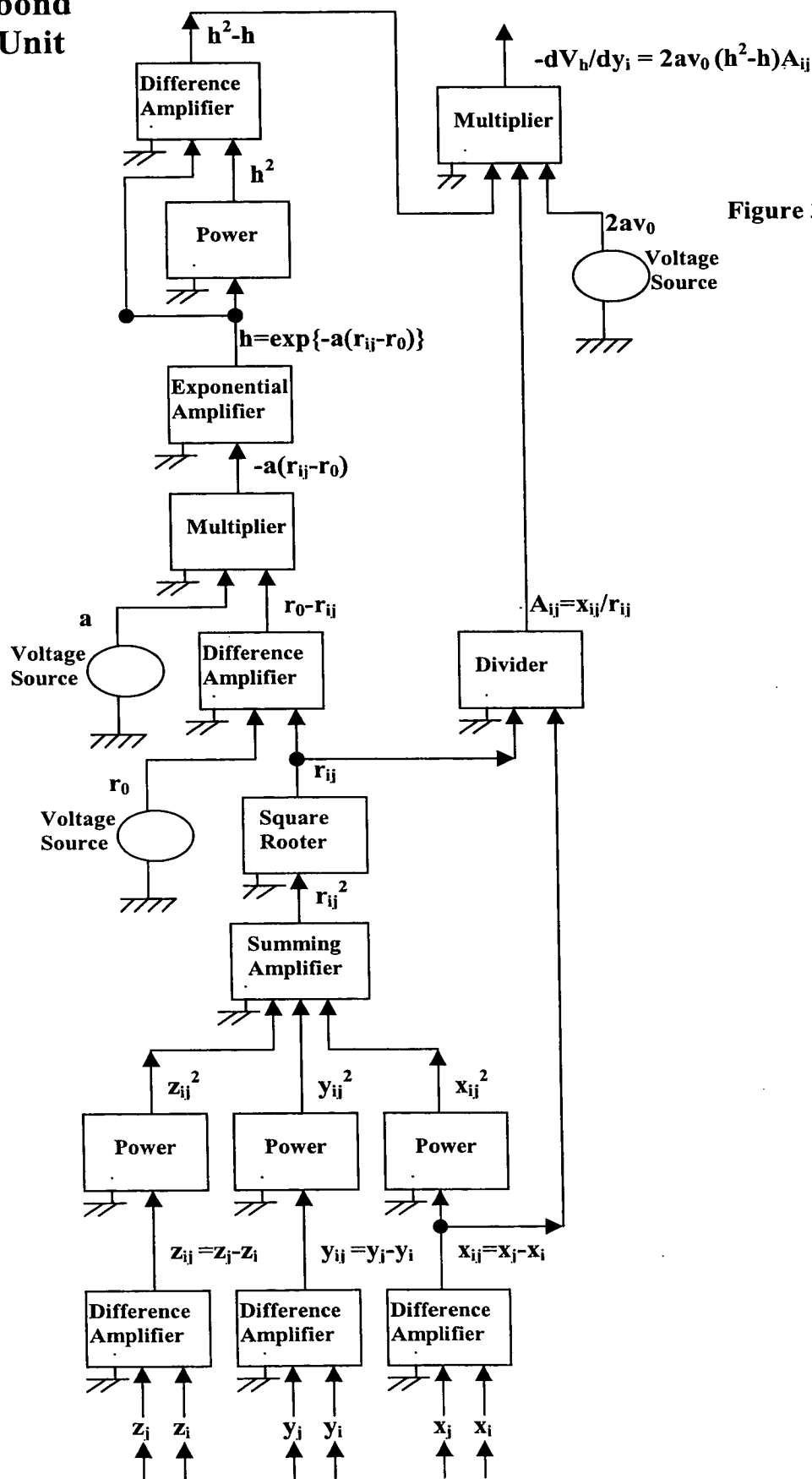


Figure 39

H-bond Z Unit

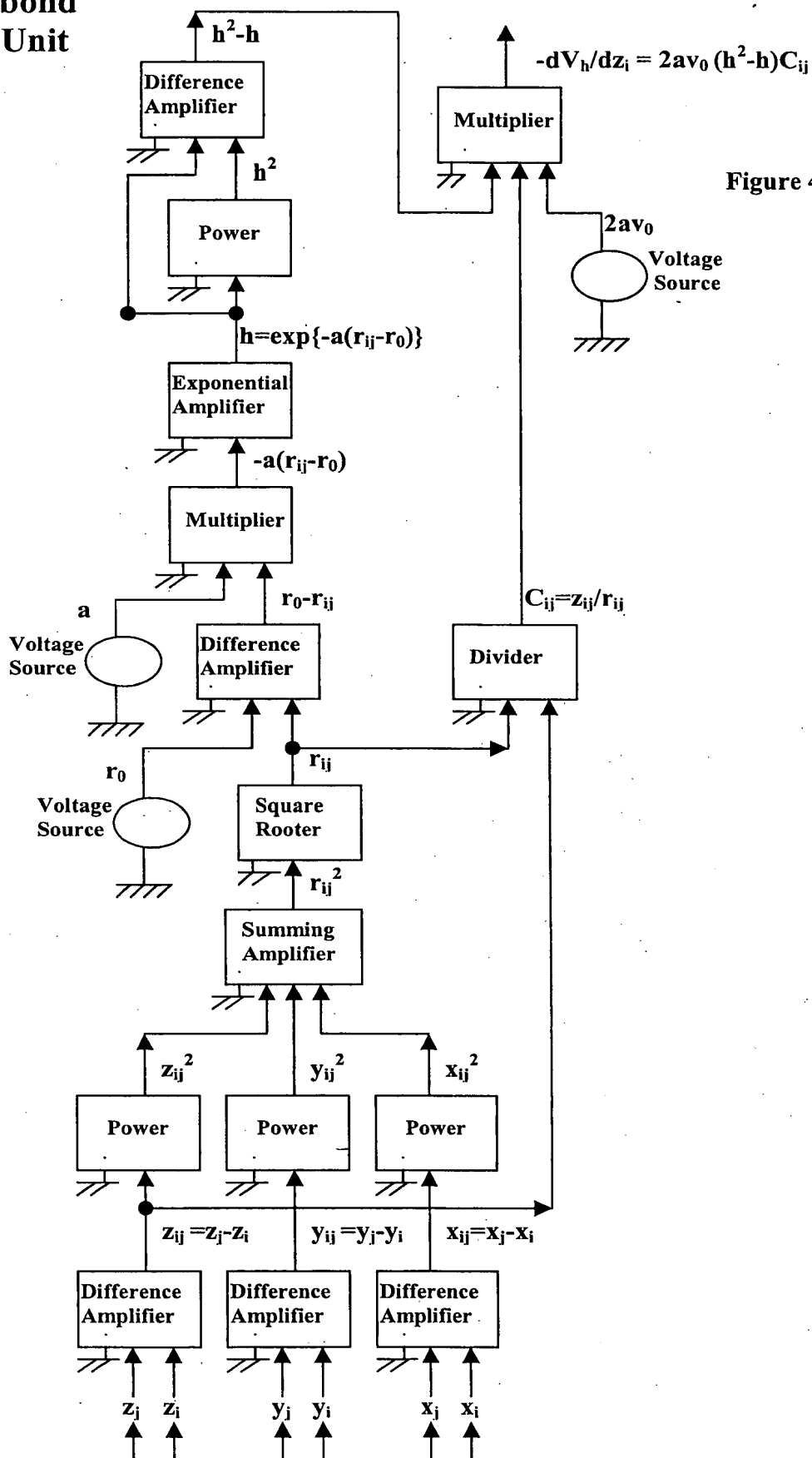


Figure 40

rABC Unit

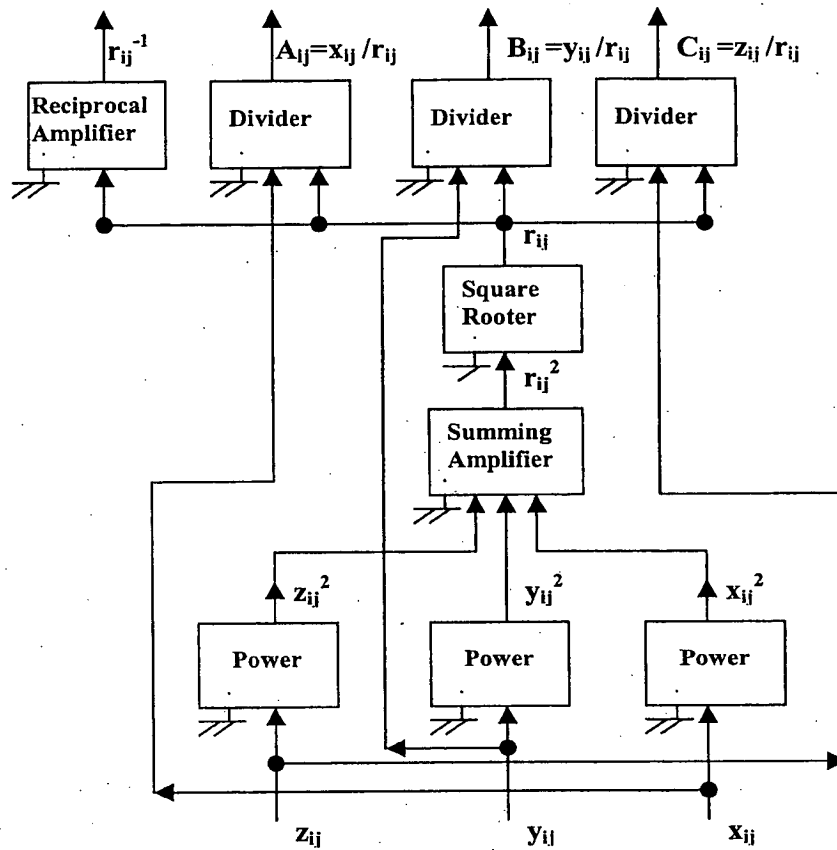
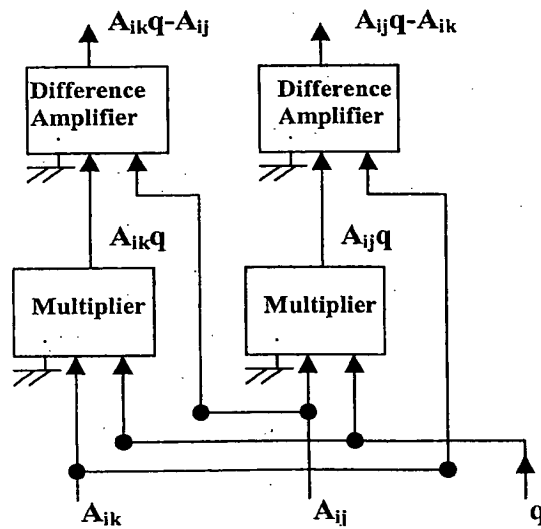


Figure 41

AqA Unit



Ua Unit

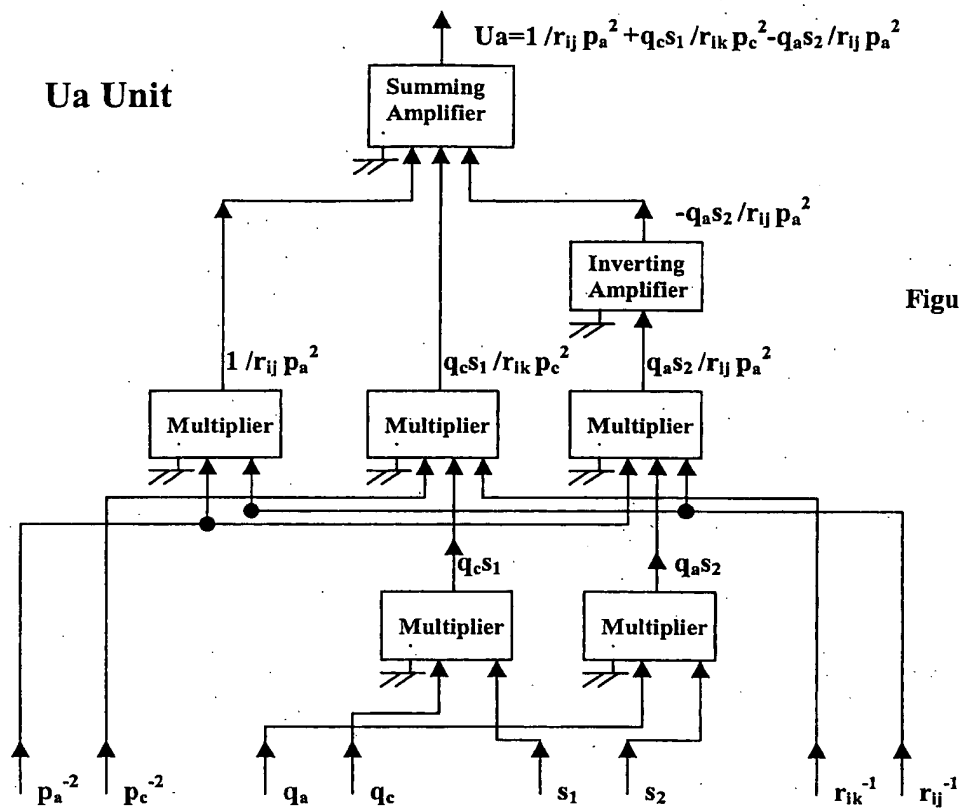
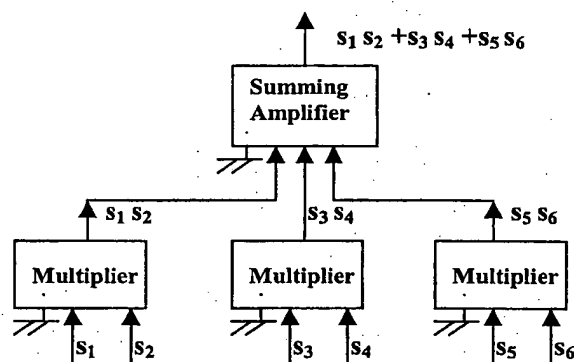
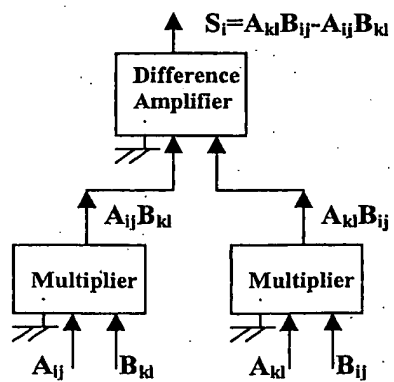


Figure 42

ss Unit



si Unit



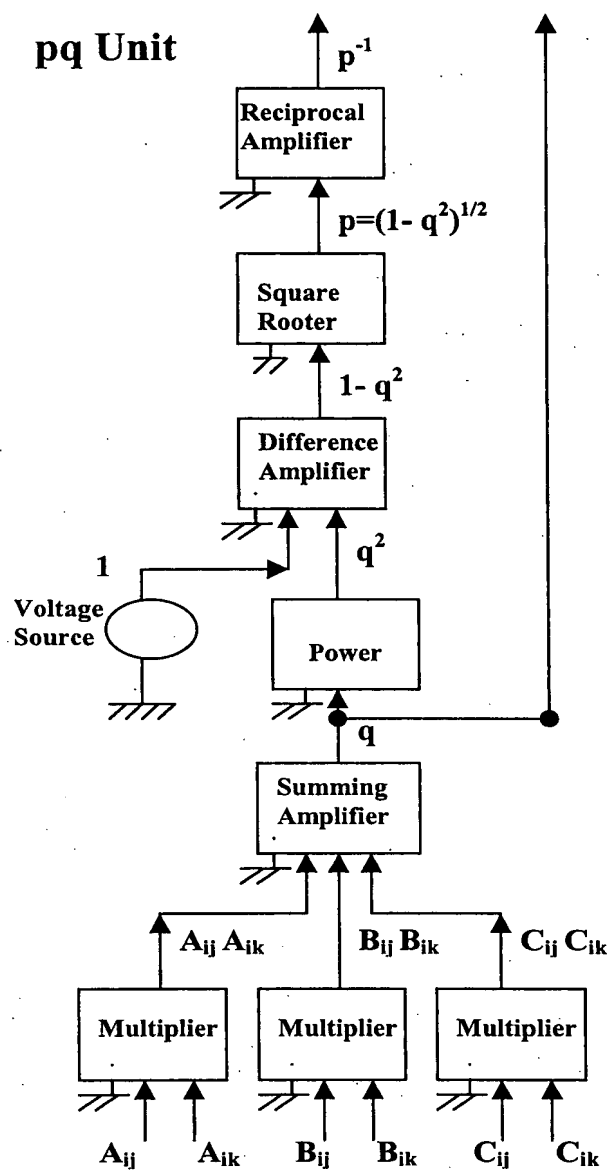


Figure 43

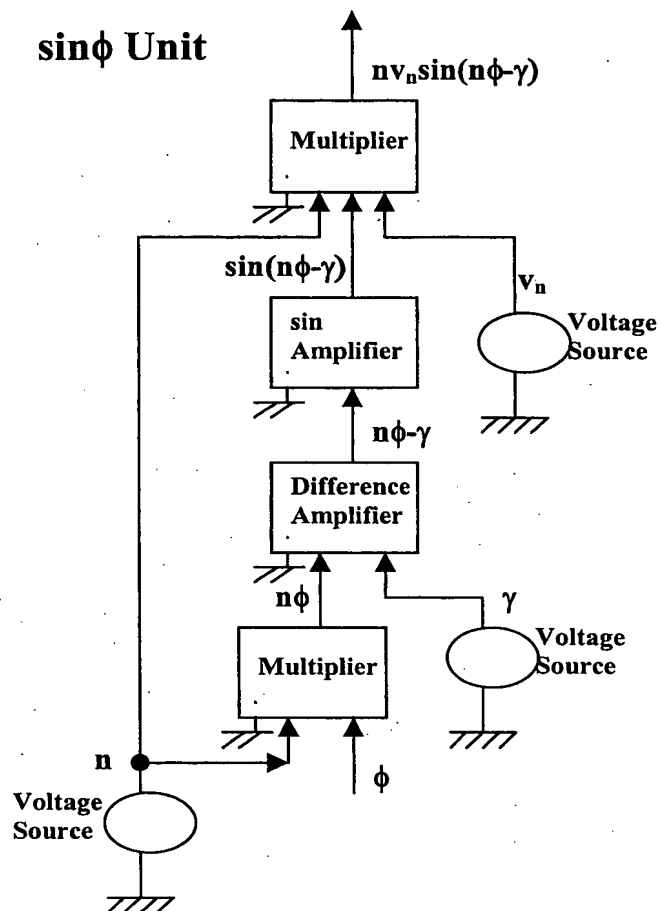


Figure 44

